



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 13, 2022 – 03:55 PM EDT

PDB ID : 8CVL
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with mRNA, aminoacylated A-site Phe-NH-tRNA^{phe}, peptidyl P-site fMTTHSMRC-NH-tRNA^{met}, and deacylated E-site tRNA^{phe} at 2.30Å resolution
Authors : Syroegin, E.A.; Aleksandrova, E.V.; Polikanov, Y.S.
Deposited on : 2022-05-18
Resolution : 2.30 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:

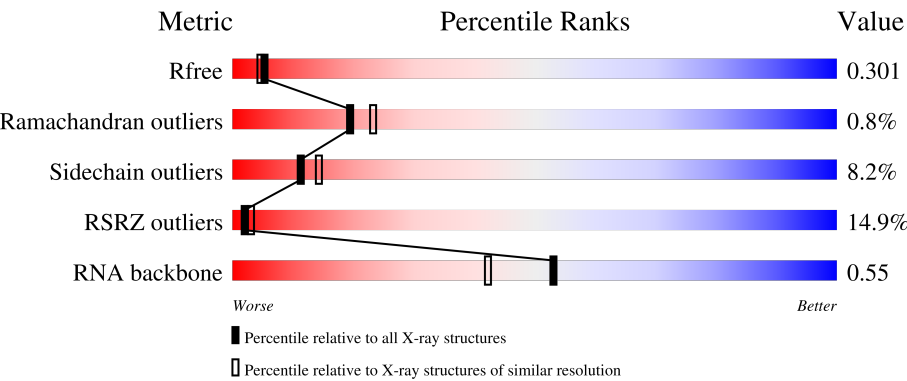
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)
RNA backbone	3102	1090 (2.70-1.90)

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>6%</div><div><div></div><div>81%</div><div>16%</div><div>..</div></div></div>
1	2A	2915	<div><div>7%</div><div><div></div><div>80%</div><div>16%</div><div>.</div></div></div>
2	1B	121	<div><div></div><div><div></div><div>91%</div><div>8%</div><div>.</div></div></div>
2	2B	121	<div><div>7%</div><div><div></div><div>80%</div><div>19%</div><div>.</div></div></div>

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Mol	Chain	Length	Quality of chain
3	1D	276	<div> <div>4%</div> <div>96%</div> <div>.</div> </div>
3	2D	276	<div> <div>12%</div> <div>96%</div> <div>.</div> </div>
4	1E	206	<div> <div>9%</div> <div>94%</div> <div>5% .</div> </div>
4	2E	206	<div> <div>7%</div> <div>93%</div> <div>6% .</div> </div>
5	1F	210	<div> <div>5%</div> <div>90%</div> <div>7% .</div> </div>
5	2F	210	<div> <div>9%</div> <div>90%</div> <div>6% .</div> </div>
6	1G	182	<div> <div>4%</div> <div>92%</div> <div>8% .</div> </div>
6	2G	182	<div> <div>16%</div> <div>88%</div> <div>10% ..</div> </div>
7	1H	180	<div> <div>6%</div> <div>92%</div> <div>. .</div> </div>
7	2H	180	<div> <div>67%</div> <div>90%</div> <div>7% .</div> </div>
8	1I	148	<div> <div>11%</div> <div>86%</div> <div>13% .</div> </div>
8	2I	148	<div> <div>28%</div> <div>84%</div> <div>14% ..</div> </div>
9	1N	140	<div> <div>14%</div> <div>94%</div> <div>6%</div> </div>
9	2N	140	<div> <div>16%</div> <div>94%</div> <div>6%</div> </div>
10	1O	122	<div> <div>3%</div> <div>97%</div> <div>.</div> </div>
10	2O	122	<div> <div>4%</div> <div>98%</div> <div>.</div> </div>
11	1P	150	<div> <div>5%</div> <div>93%</div> <div>6% .</div> </div>
11	2P	150	<div> <div>24%</div> <div>88%</div> <div>11% .</div> </div>
12	1Q	141	<div> <div>5%</div> <div>95%</div> <div>5%</div> </div>
12	2Q	141	<div> <div>30%</div> <div>99%</div> <div>.</div> </div>
13	1R	118	<div> <div>5%</div> <div>94%</div> <div>6%</div> </div>
13	2R	118	<div> <div>8%</div> <div>94%</div> <div>6%</div> </div>
14	1S	112	<div> <div>3%</div> <div>95%</div> <div>. .</div> </div>
14	2S	112	<div> <div>16%</div> <div>90%</div> <div>7% ..</div> </div>
15	1T	146	<div> <div>5%</div> <div>86%</div> <div>. 10%</div> </div>



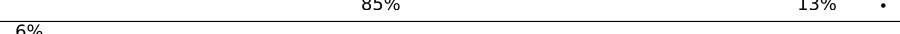


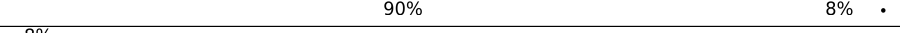

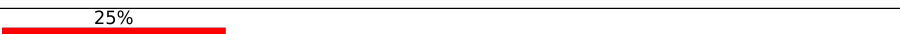
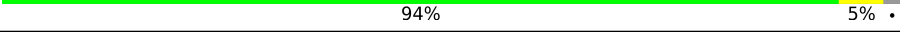
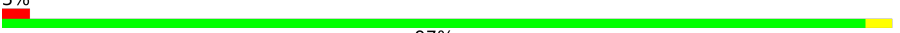
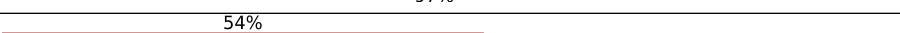
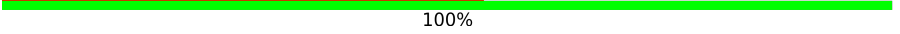

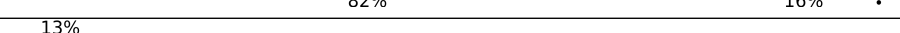


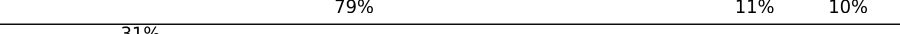








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Mol	Chain	Length	Quality of chain
15	2T	146	
16	1U	118	
16	2U	118	
17	1V	101	
17	2V	101	
18	1W	113	
18	2W	113	
19	1X	96	
19	2X	96	
20	1Y	110	
20	2Y	110	
21	1Z	206	
21	2Z	206	
22	10	85	
22	20	85	
23	11	98	
23	21	98	
24	12	72	
24	22	72	
25	13	60	
25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

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Mol	Chain	Length	Quality of chain
28	16	54	
28	26	54	
29	17	49	
29	27	49	
30	18	65	
30	28	65	
31	19	37	
31	29	37	
32	1a	1521	
32	2a	1521	
33	1b	256	
33	2b	256	
34	1c	239	
34	2c	239	
35	1d	209	
35	2d	209	
36	1e	162	
36	2e	162	
37	1f	101	
37	2f	101	
38	1g	156	
38	2g	156	
39	1h	138	
39	2h	138	
40	1i	128	

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Mol	Chain	Length	Quality of chain
40	2i	128	
41	1j	105	
41	2j	105	
42	1k	129	
42	2k	129	
43	1l	132	
43	2l	132	
44	1m	126	
44	2m	126	
45	1n	61	
45	2n	61	
46	1o	89	
46	2o	89	
47	1p	88	
47	2p	88	
48	1q	105	
48	2q	105	
49	1r	88	
49	2r	88	
50	1s	93	
50	2s	93	
51	1t	106	
51	2t	106	
52	1u	27	
52	2u	27	

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Mol	Chain	Length	Quality of chain
53	1v	24	
53	2v	24	
54	1w	76	
54	2w	76	
55	1x	77	
55	2x	77	
56	1z	7	
56	2z	7	
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
56	FME	1z	1	-	-	-	X
56	FME	2z	1	-	-	-	X
57	PSU	1y	32	-	-	-	X
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
57	4SU	2y	8	-	-	-	X
58	MG	18	107	-	-	-	X
58	MG	1A	3308	-	-	-	X
58	MG	1A	3351	-	-	-	X
58	MG	1A	3406	-	-	-	X
58	MG	1A	3409	-	-	-	X
58	MG	1A	3432	-	-	-	X
58	MG	1A	3601	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	MG	1A	3947	-	-	-	X
58	MG	1A	3976	-	-	-	X
58	MG	1O	201	-	-	-	X
58	MG	1a	1742	-	-	-	X
58	MG	20	101	-	-	-	X
58	MG	25	103	-	-	-	X
58	MG	2A	3160	-	-	-	X
58	MG	2A	3195	-	-	-	X
58	MG	2A	3197	-	-	-	X
58	MG	2A	3257	-	-	-	X
58	MG	2A	3289	-	-	-	X
58	MG	2A	3293	-	-	-	X
58	MG	2A	3296	-	-	-	X
58	MG	2A	3340	-	-	-	X
58	MG	2A	3384	-	-	-	X
58	MG	2A	3640	-	-	-	X
58	MG	2A	3759	-	-	-	X
58	MG	2A	3777	-	-	-	X
58	MG	2A	3837	-	-	-	X
58	MG	2B	202	-	-	-	X
58	MG	2R	204	-	-	-	X
58	MG	2a	1640	-	-	-	X

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 299898 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 fMTHSMRC-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 fMTHSMRC-NH-tRNA_{met} Peptide-part.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	1z	7	Total	C	N	O	S	0	0	0
			58	33	12	10	3			
56	2z	7	Total	C	N	O	S	0	0	0
			58	33	12	10	3			

- 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	1101	Total Mg 1101 1101	0	0
58	1B	38	Total Mg 38 38	0	0
58	1D	13	Total Mg 13 13	0	0
58	1E	12	Total Mg 12 12	0	0
58	1F	12	Total Mg 12 12	0	0
58	1G	5	Total Mg 5 5	0	0
58	1H	1	Total Mg 1 1	0	0
58	1I	1	Total Mg 1 1	0	0
58	1N	5	Total Mg 5 5	0	0
58	1O	5	Total Mg 5 5	0	0
58	1P	7	Total Mg 7 7	0	0
58	1Q	8	Total Mg 8 8	0	0
58	1R	4	Total Mg 4 4	0	0
58	1S	3	Total Mg 3 3	0	0
58	1T	2	Total Mg 2 2	0	0
58	1U	10	Total Mg 10 10	0	0
58	1V	7	Total Mg 7 7	0	0
58	1W	4	Total Mg 4 4	0	0
58	1X	4	Total Mg 4 4	0	0
58	1Y	4	Total Mg 4 4	0	0
58	1Z	4	Total Mg 4 4	0	0
58	10	9	Total Mg 9 9	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	11	6	Total 6	Mg 6	0	0
58	12	2	Total 2	Mg 2	0	0
58	13	4	Total 4	Mg 4	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	5	Total 5	Mg 5	0	0
58	18	7	Total 7	Mg 7	0	0
58	19	1	Total 1	Mg 1	0	0
58	1a	210	Total 210	Mg 210	0	0
58	1b	1	Total 1	Mg 1	0	0
58	1d	1	Total 1	Mg 1	0	0
58	1e	2	Total 2	Mg 2	0	0
58	1f	2	Total 2	Mg 2	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	1w	7	Total 7	Mg 7	0	0
58	1x	12	Total 12	Mg 12	0	0
58	2A	851	Total 851	Mg 851	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	2B	20	Total 20	Mg 20	0	0
58	2D	7	Total 7	Mg 7	0	0
58	2E	10	Total 10	Mg 10	0	0
58	2F	6	Total 6	Mg 6	0	0
58	2G	1	Total 1	Mg 1	0	0
58	2N	1	Total 1	Mg 1	0	0
58	2O	2	Total 2	Mg 2	0	0
58	2P	2	Total 2	Mg 2	0	0
58	2Q	4	Total 4	Mg 4	0	0
58	2R	4	Total 4	Mg 4	0	0
58	2T	4	Total 4	Mg 4	0	0
58	2U	1	Total 1	Mg 1	0	0
58	2V	2	Total 2	Mg 2	0	0
58	2W	1	Total 1	Mg 1	0	0
58	2X	1	Total 1	Mg 1	0	0
58	2Y	1	Total 1	Mg 1	0	0
58	2Z	1	Total 1	Mg 1	0	0
58	20	2	Total 2	Mg 2	0	0
58	21	1	Total 1	Mg 1	0	0
58	23	3	Total 3	Mg 3	0	0
58	25	3	Total 3	Mg 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	27	2	Total 2	Mg 2	0	0
58	28	4	Total 4	Mg 4	0	0
58	29	1	Total 1	Mg 1	0	0
58	2a	220	Total 220	Mg 220	0	0
58	2d	3	Total 3	Mg 3	0	0
58	2e	1	Total 1	Mg 1	0	0
58	2f	2	Total 2	Mg 2	0	0
58	2i	1	Total 1	Mg 1	0	0
58	2j	2	Total 2	Mg 2	0	0
58	2k	1	Total 1	Mg 1	0	0
58	2l	3	Total 3	Mg 3	0	0
58	2n	1	Total 1	Mg 1	0	0
58	2q	3	Total 3	Mg 3	0	0
58	2r	1	Total 1	Mg 1	0	0
58	2t	2	Total 2	Mg 2	0	0
58	2v	4	Total 4	Mg 4	0	0
58	2w	4	Total 4	Mg 4	0	0
58	2x	6	Total 6	Mg 6	0	0

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

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

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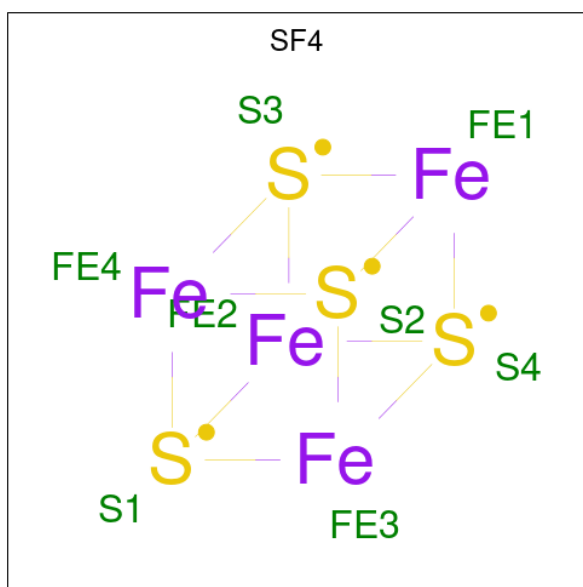
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	2A	1	Total K 1 1	0	0

- 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	1949	Total	O	0	0
			1949	1949		
62	1B	58	Total	O	0	0
			58	58		
62	1D	26	Total	O	0	0
			26	26		
62	1E	28	Total	O	0	0
			28	28		
62	1F	18	Total	O	0	0
			18	18		
62	1G	3	Total	O	0	0
			3	3		
62	1H	2	Total	O	0	0
			2	2		
62	1N	6	Total	O	0	0
			6	6		
62	1O	6	Total	O	0	0
			6	6		
62	1P	19	Total	O	0	0
			19	19		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	1Q	7	Total 7	O 7	0	0
62	1R	10	Total 10	O 10	0	0
62	1S	4	Total 4	O 4	0	0
62	1T	7	Total 7	O 7	0	0
62	1U	13	Total 13	O 13	0	0
62	1V	9	Total 9	O 9	0	0
62	1W	7	Total 7	O 7	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	13	Total 13	O 13	0	0
62	11	7	Total 7	O 7	0	0
62	12	3	Total 3	O 3	0	0
62	13	6	Total 6	O 6	0	0
62	15	8	Total 8	O 8	0	0
62	16	2	Total 2	O 2	0	0
62	17	8	Total 8	O 8	0	0
62	18	12	Total 12	O 12	0	0
62	1a	301	Total 301	O 301	0	0
62	1b	1	Total 1	O 1	0	0
62	1e	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	1f	1	Total 1	O 1	0	0
62	1i	1	Total 1	O 1	0	0
62	1l	5	Total 5	O 5	0	0
62	1m	1	Total 1	O 1	0	0
62	1o	2	Total 2	O 2	0	0
62	1q	2	Total 2	O 2	0	0
62	1v	5	Total 5	O 5	0	0
62	1w	9	Total 9	O 9	0	0
62	1x	7	Total 7	O 7	0	0
62	1z	3	Total 3	O 3	0	0
62	2A	1047	Total 1047	O 1047	0	0
62	2B	20	Total 20	O 20	0	0
62	2D	26	Total 26	O 26	0	0
62	2E	15	Total 15	O 15	0	0
62	2F	14	Total 14	O 14	0	0
62	2N	1	Total 1	O 1	0	0
62	2O	2	Total 2	O 2	0	0
62	2P	10	Total 10	O 10	0	0
62	2Q	2	Total 2	O 2	0	0
62	2R	3	Total 3	O 3	0	0
62	2T	6	Total 6	O 6	0	0

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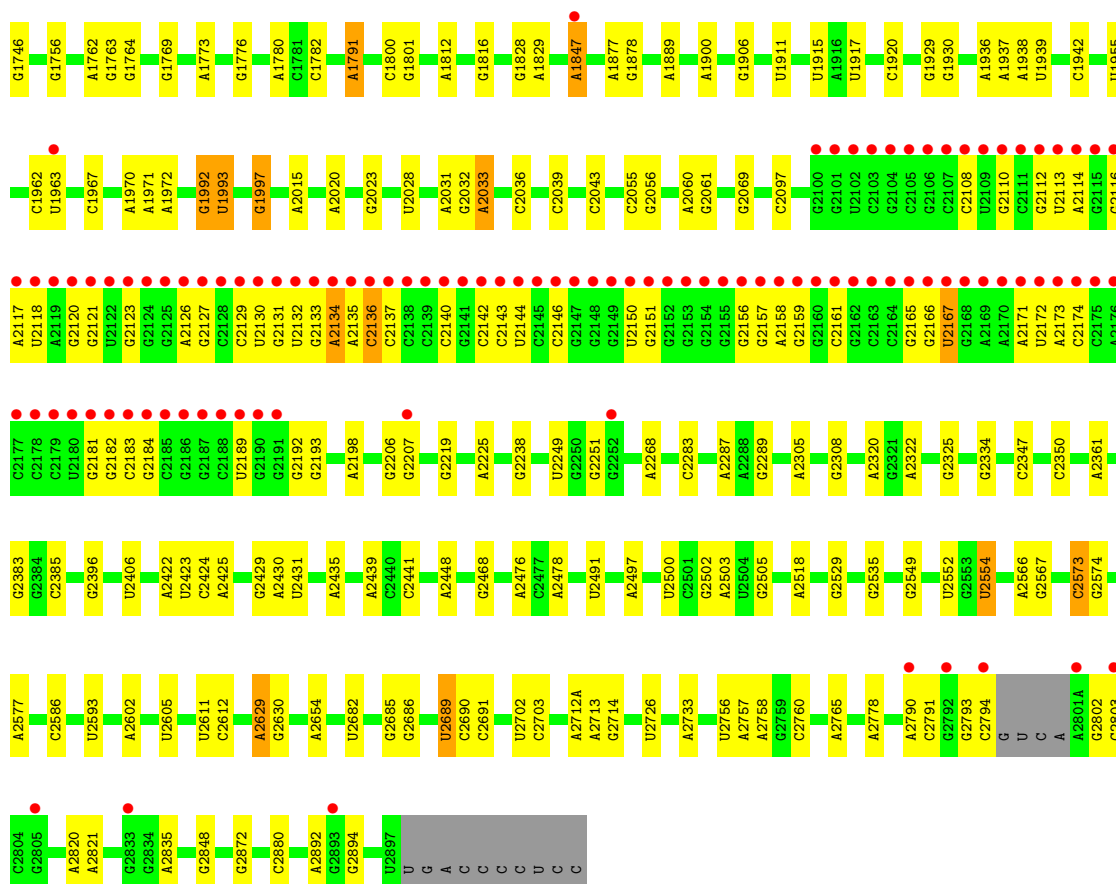
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	2U	1	Total 1	O 1	0	0
62	2V	1	Total 1	O 1	0	0
62	2W	3	Total 3	O 3	0	0
62	2X	5	Total 5	O 5	0	0
62	20	2	Total 2	O 2	0	0
62	21	7	Total 7	O 7	0	0
62	22	1	Total 1	O 1	0	0
62	23	2	Total 2	O 2	0	0
62	25	2	Total 2	O 2	0	0
62	27	5	Total 5	O 5	0	0
62	28	3	Total 3	O 3	0	0
62	29	1	Total 1	O 1	0	0
62	2a	196	Total 196	O 196	0	0
62	2c	1	Total 1	O 1	0	0
62	2d	1	Total 1	O 1	0	0
62	2e	2	Total 2	O 2	0	0
62	2g	1	Total 1	O 1	0	0
62	2i	1	Total 1	O 1	0	0
62	2j	2	Total 2	O 2	0	0
62	2l	5	Total 5	O 5	0	0
62	2r	1	Total 1	O 1	0	0

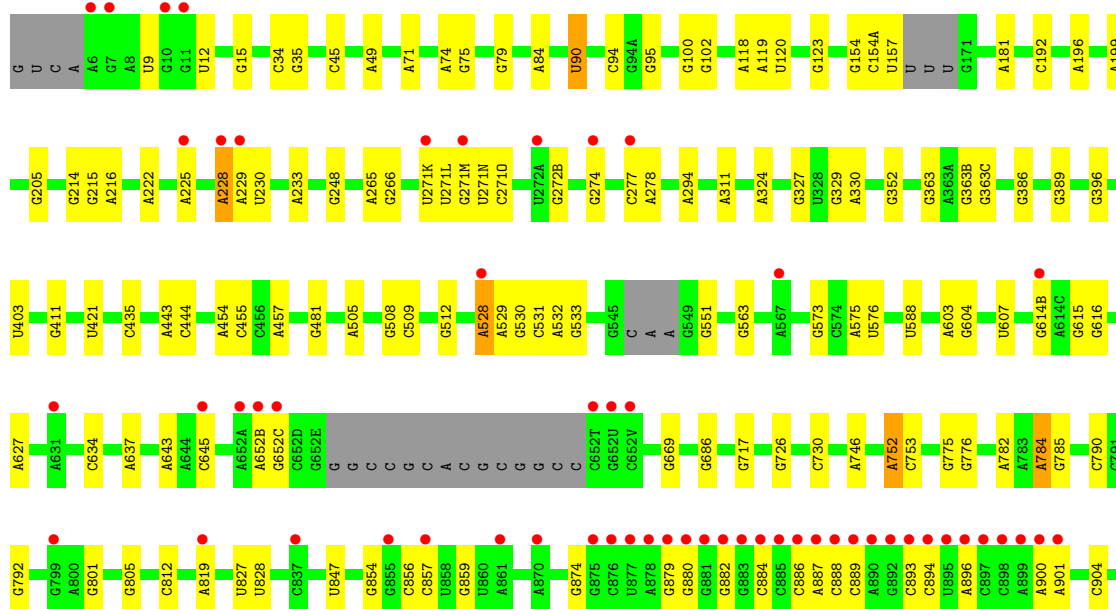
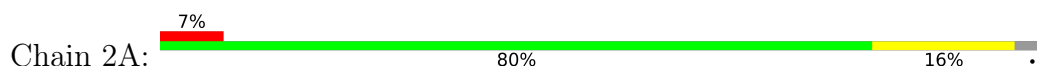
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	2t	1	Total	O	0	0
			1	1		
62	2v	2	Total	O	0	0
			2	2		
62	2w	6	Total	O	0	0
			6	6		
62	2x	4	Total	O	0	0
			4	4		
62	2z	1	Total	O	0	0
			1	1		



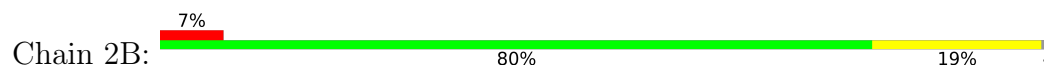
• Molecule 1: 23S Ribosomal RNA



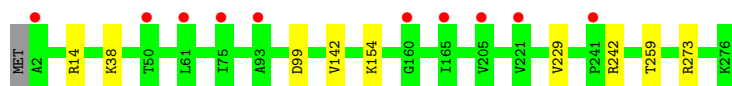




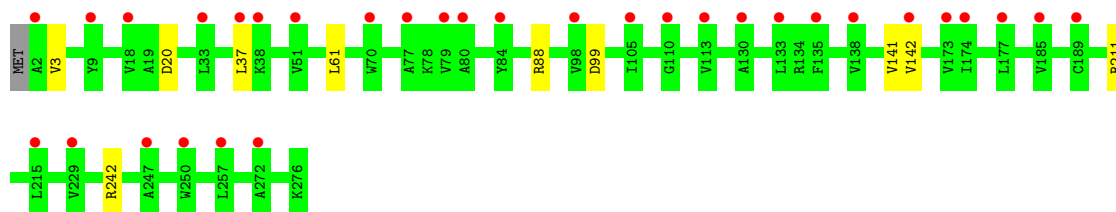
- Molecule 2: 5S Ribosomal RNA



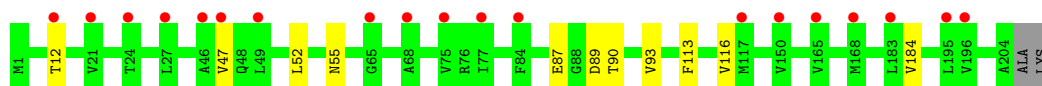
- Molecule 3: 50S ribosomal protein L2



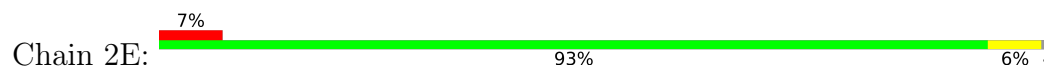
- Molecule 3: 50S ribosomal protein L2



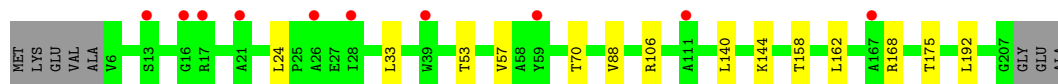
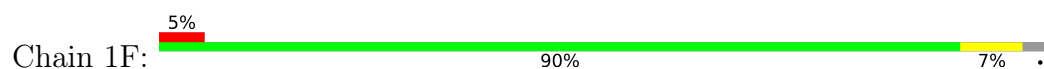
- Molecule 4: 50S ribosomal protein L3



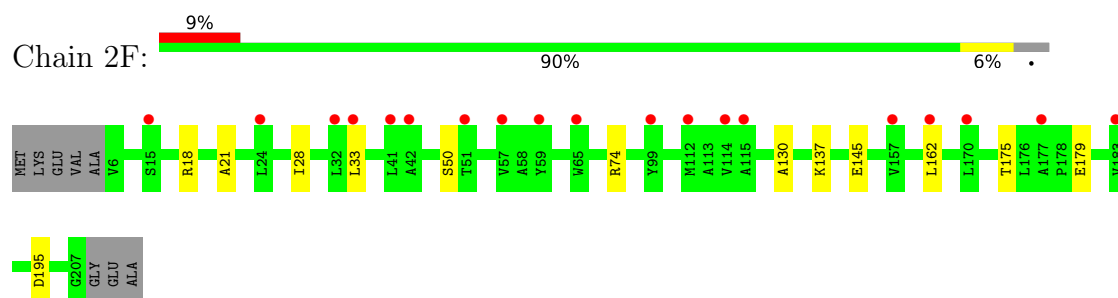
- Molecule 4: 50S ribosomal protein L3



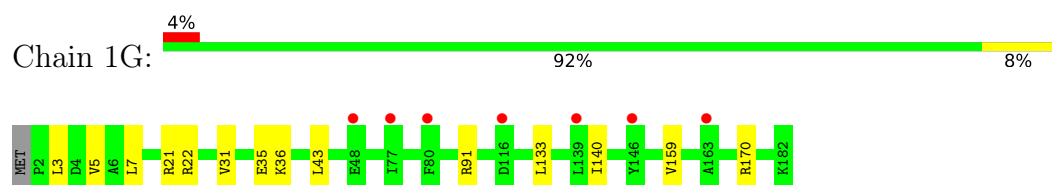
- Molecule 5: 50S ribosomal protein L4



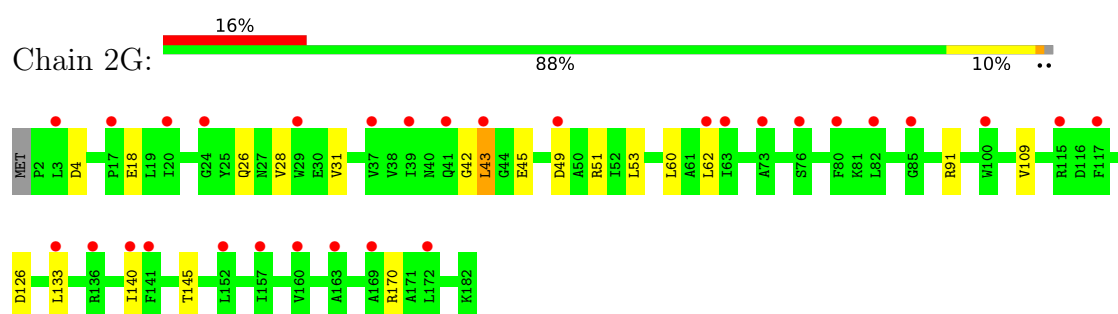
- Molecule 5: 50S ribosomal protein L4



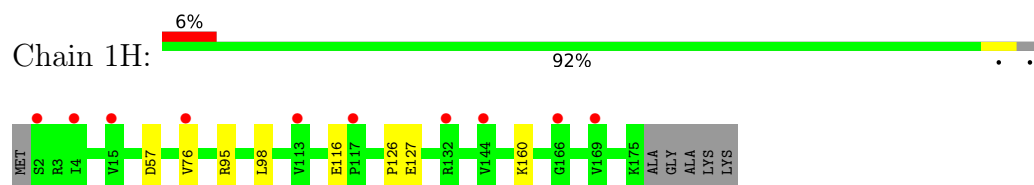
- Molecule 6: 50S ribosomal protein L5



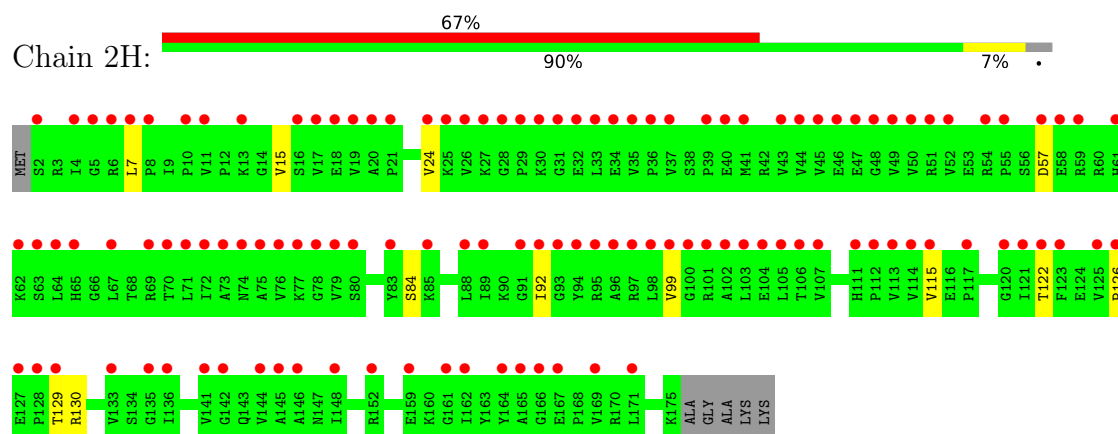
- Molecule 6: 50S ribosomal protein L5



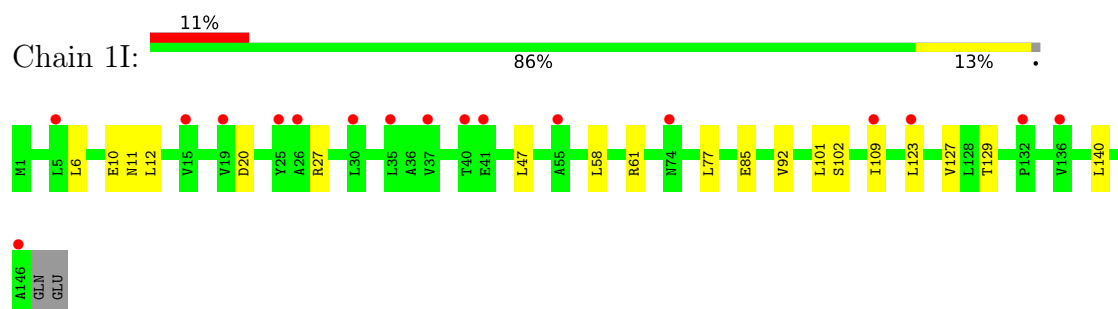
- Molecule 7: 50S ribosomal protein L6



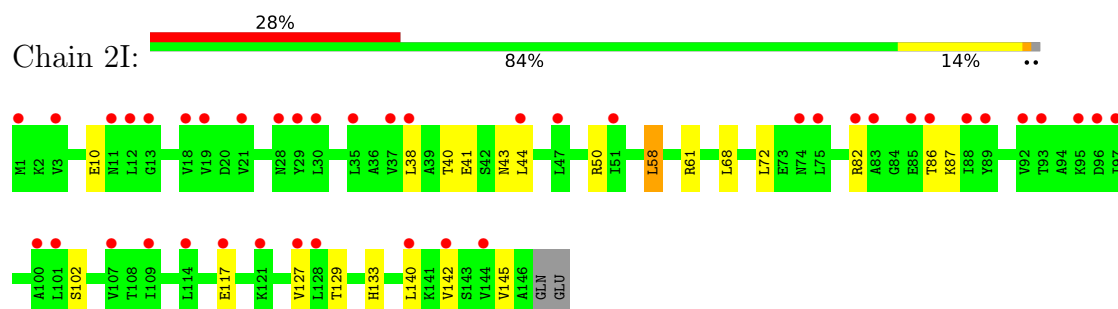
- Molecule 7: 50S ribosomal protein L6



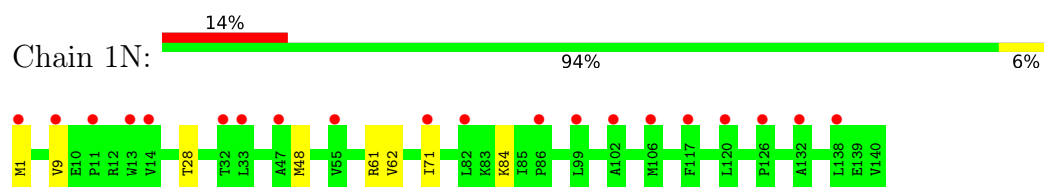
- Molecule 8: 50S ribosomal protein L9



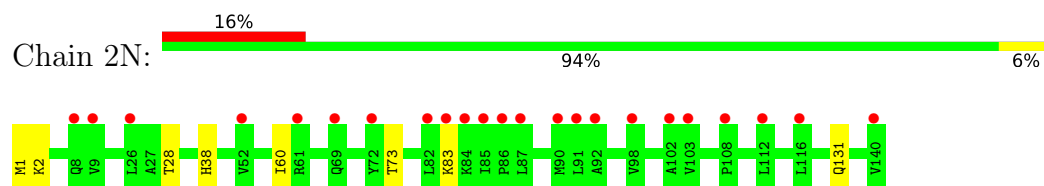
- Molecule 8: 50S ribosomal protein L9



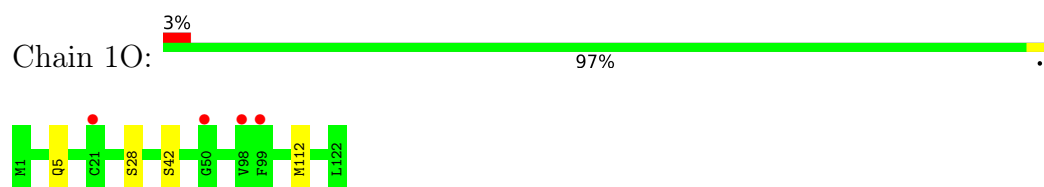
- Molecule 9: 50S ribosomal protein L13



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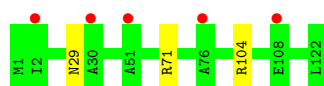


- Molecule 10: 50S ribosomal protein L14



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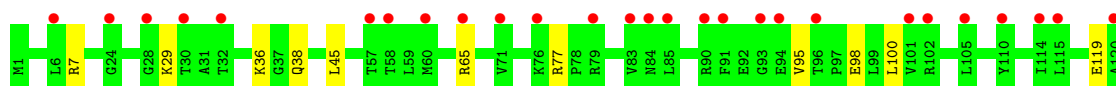
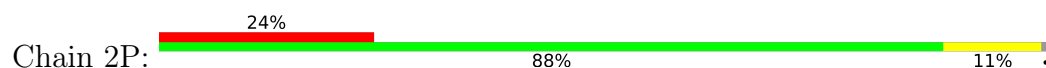




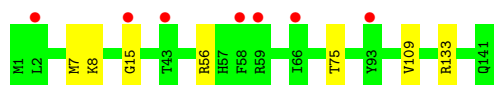
- Molecule 11: 50S ribosomal protein L15



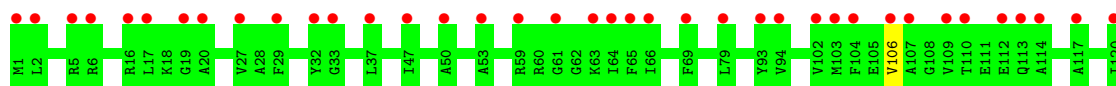
- Molecule 11: 50S ribosomal protein L15



- Molecule 12: 50S ribosomal protein L16



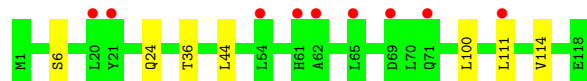
- Molecule 12: 50S ribosomal protein L16



- Molecule 13: 50S ribosomal protein L17



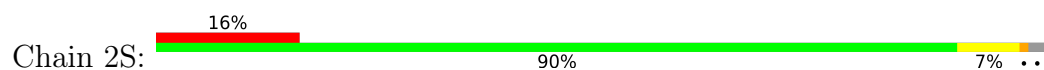
- Molecule 13: 50S ribosomal protein L17



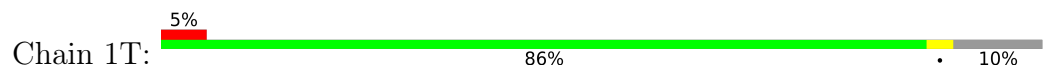
- Molecule 14: 50S ribosomal protein L18



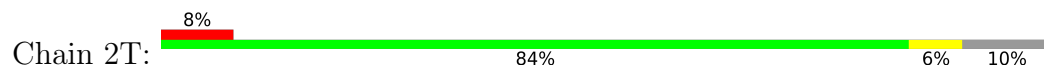
- Molecule 14: 50S ribosomal protein L18



- Molecule 15: 50S ribosomal protein L19



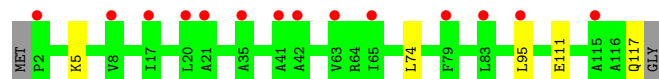
- Molecule 15: 50S ribosomal protein L19



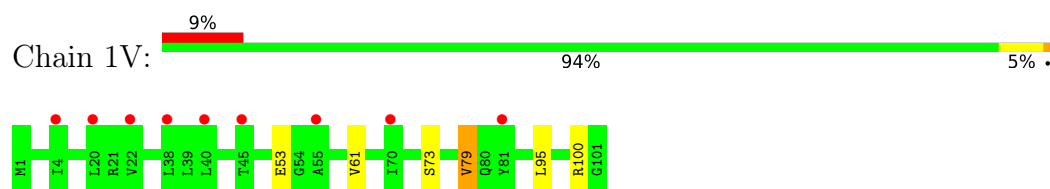
- Molecule 16: 50S ribosomal protein L20



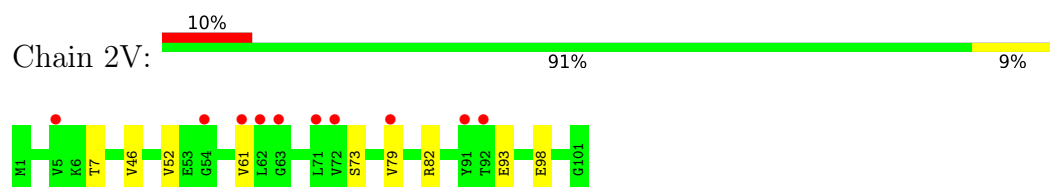
- Molecule 16: 50S ribosomal protein L20



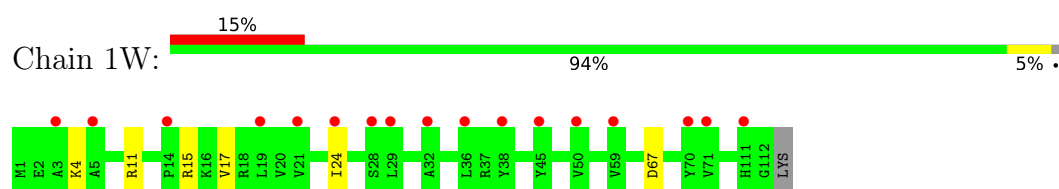
• Molecule 17: 50S ribosomal protein L21



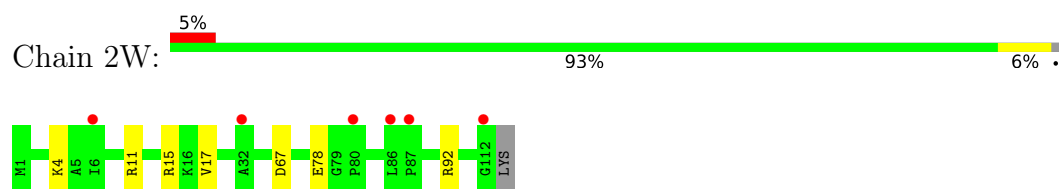
• Molecule 17: 50S ribosomal protein L21



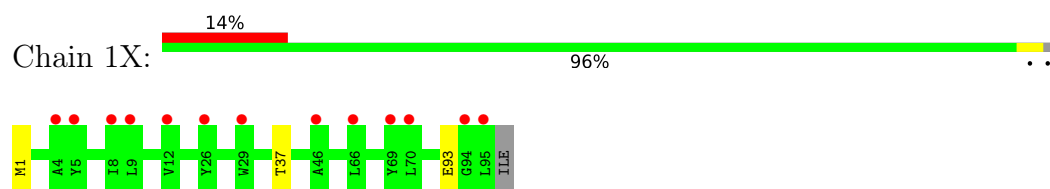
• Molecule 18: 50S ribosomal protein L22



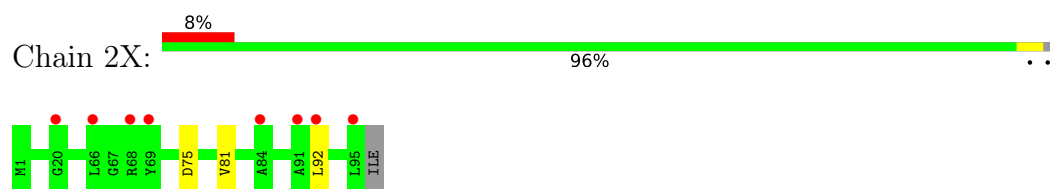
• Molecule 18: 50S ribosomal protein L22



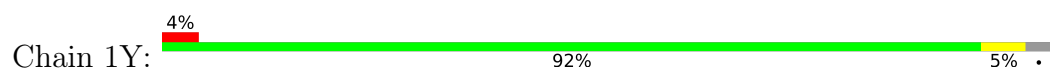
• Molecule 19: 50S ribosomal protein L23



• Molecule 19: 50S ribosomal protein L23

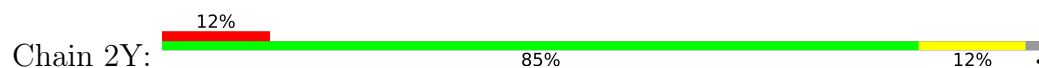


• Molecule 20: 50S ribosomal protein L24

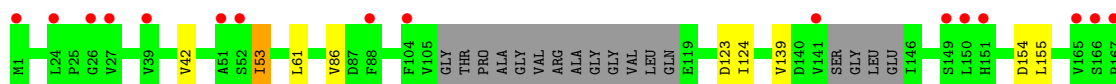




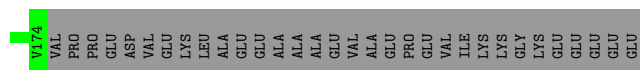
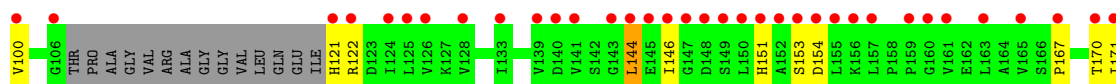
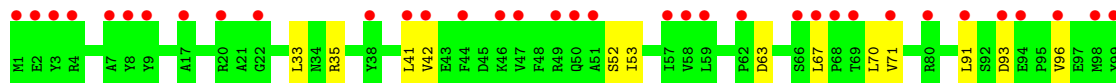
- Molecule 20: 50S ribosomal protein L24



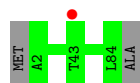
- Molecule 21: 50S ribosomal protein L25



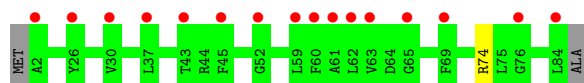
- Molecule 21: 50S ribosomal protein L25



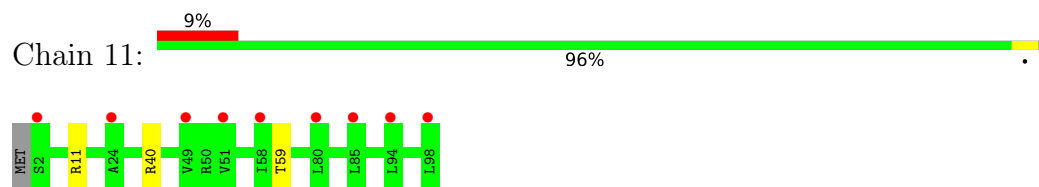
- Molecule 22: 50S ribosomal protein L27



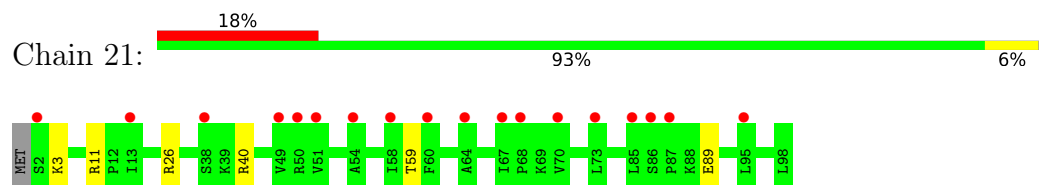
- Molecule 22: 50S ribosomal protein L27



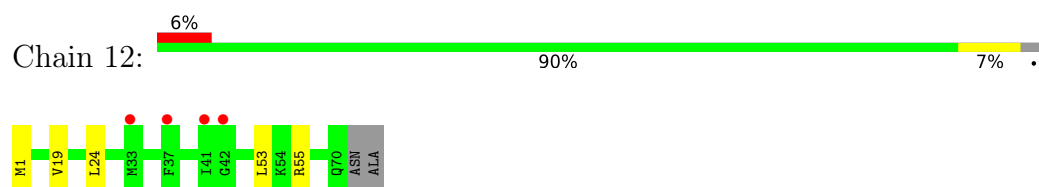
- Molecule 23: 50S ribosomal protein L28



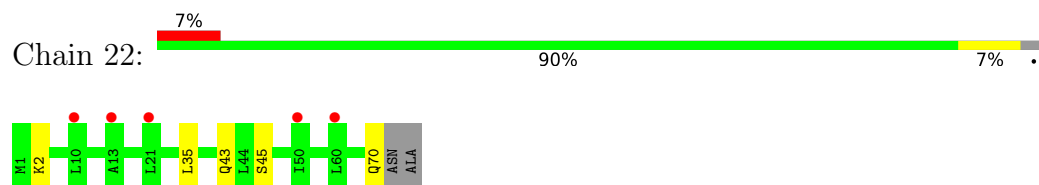
- Molecule 23: 50S ribosomal protein L28



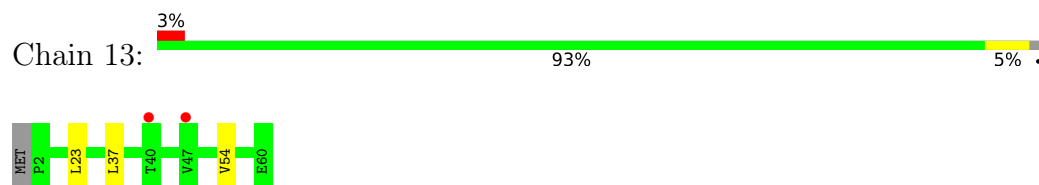
- Molecule 24: 50S ribosomal protein L29



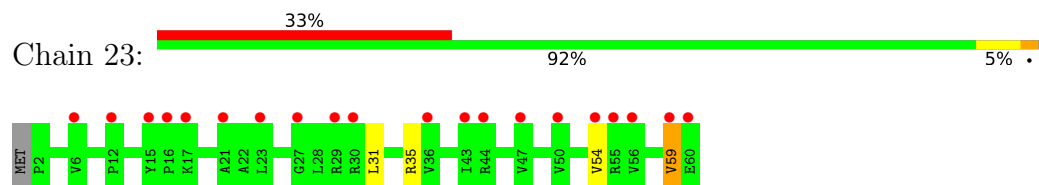
- Molecule 24: 50S ribosomal protein L29



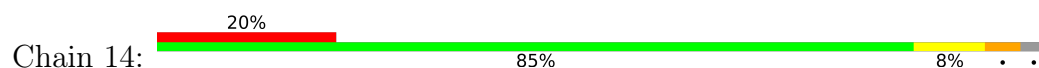
- Molecule 25: 50S ribosomal protein L30



- Molecule 25: 50S ribosomal protein L30

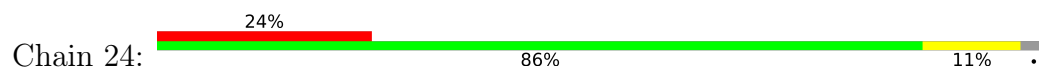


- Molecule 26: 50S ribosomal protein L31





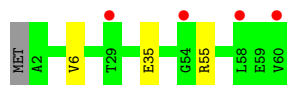
- Molecule 26: 50S ribosomal protein L31



- Molecule 27: 50S ribosomal protein L32



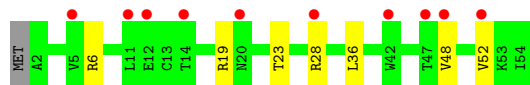
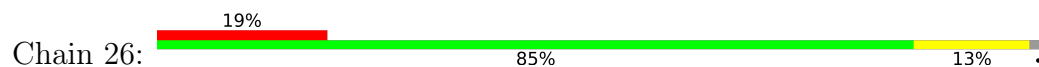
- Molecule 27: 50S ribosomal protein L32



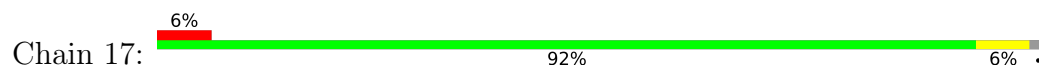
- Molecule 28: 50S ribosomal protein L33



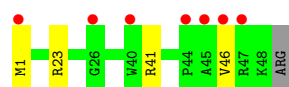
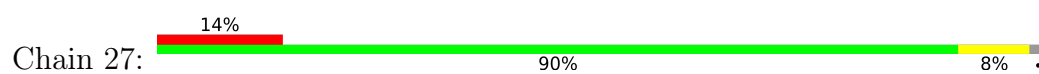
- Molecule 28: 50S ribosomal protein L33



- Molecule 29: 50S ribosomal protein L34



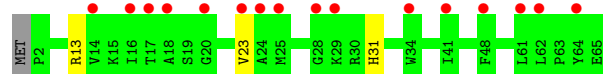
- Molecule 29: 50S ribosomal protein L34



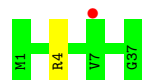
- Molecule 30: 50S ribosomal protein L35



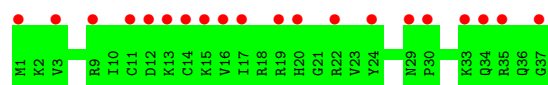
- Molecule 30: 50S ribosomal protein L35



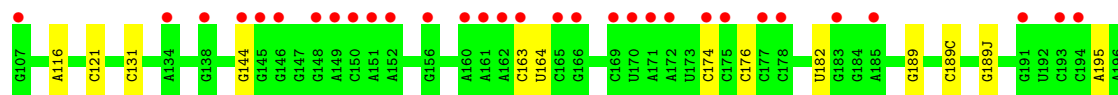
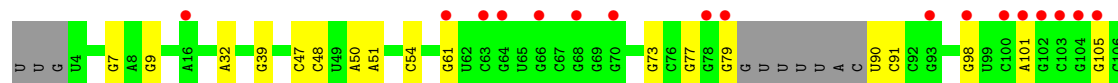
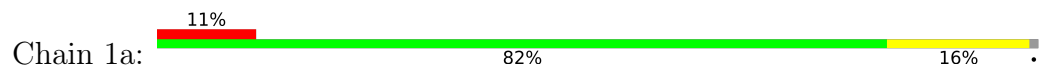
- Molecule 31: 50S ribosomal protein L36

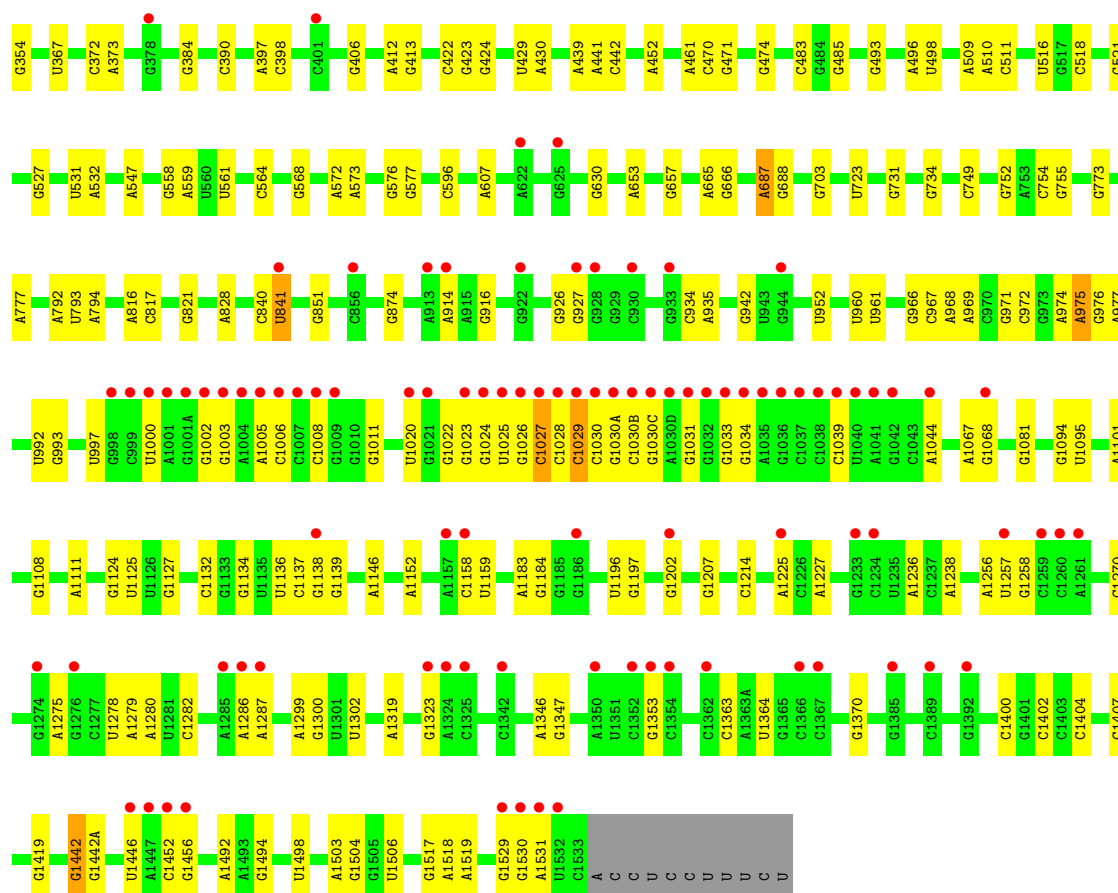


- Molecule 31: 50S ribosomal protein L36

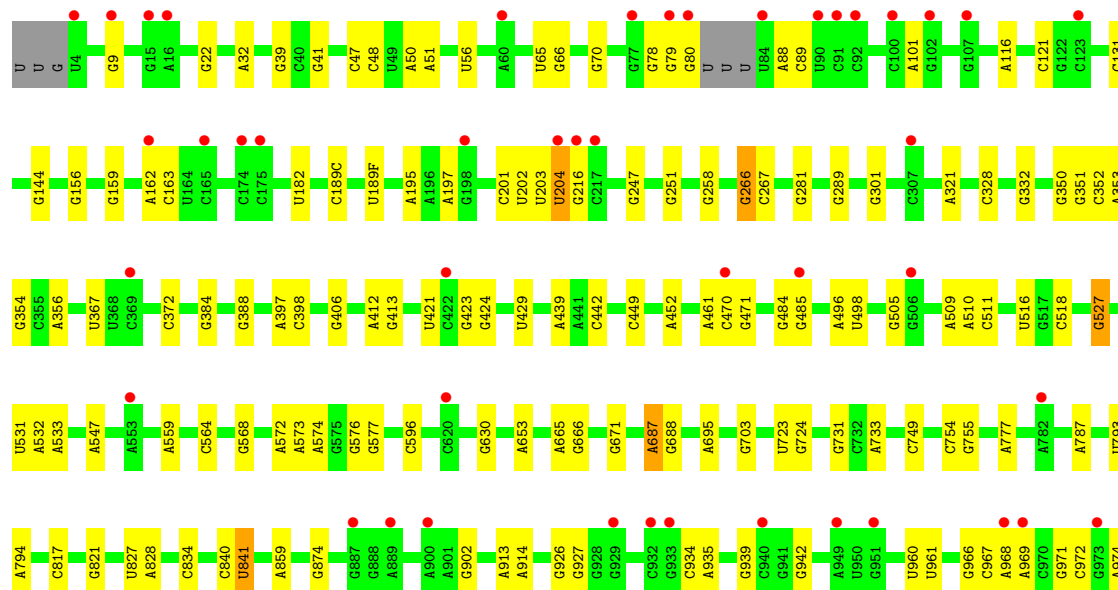
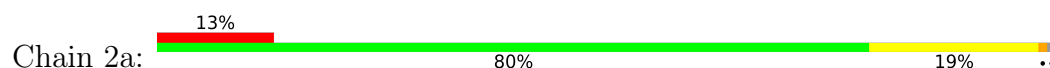


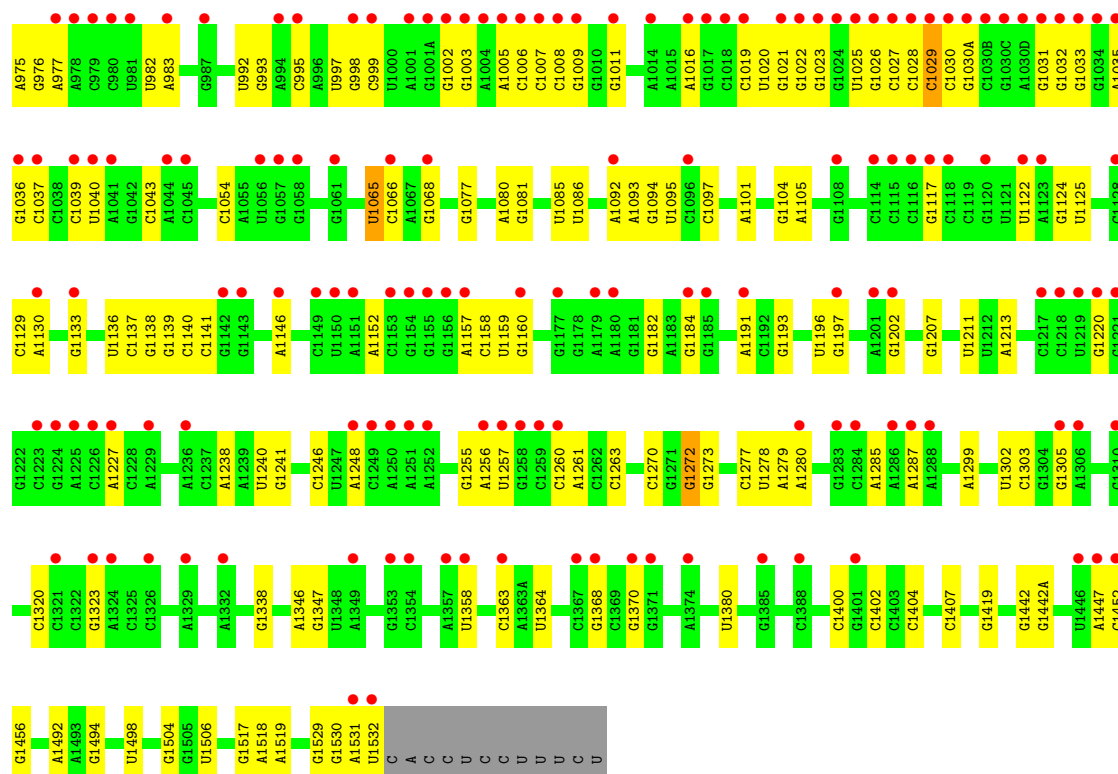
- Molecule 32: 16S Ribosomal RNA



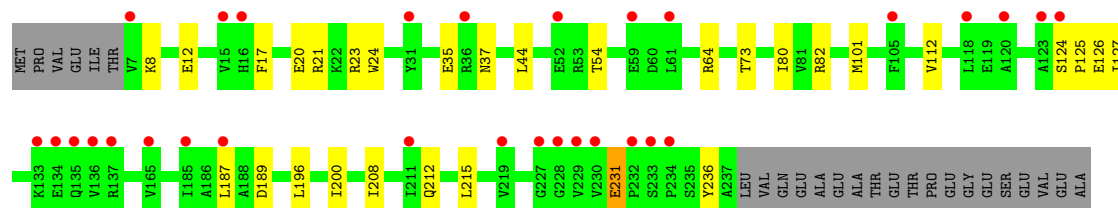
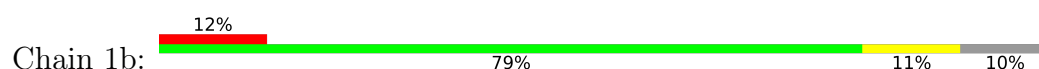


• Molecule 32: 16S Ribosomal RNA

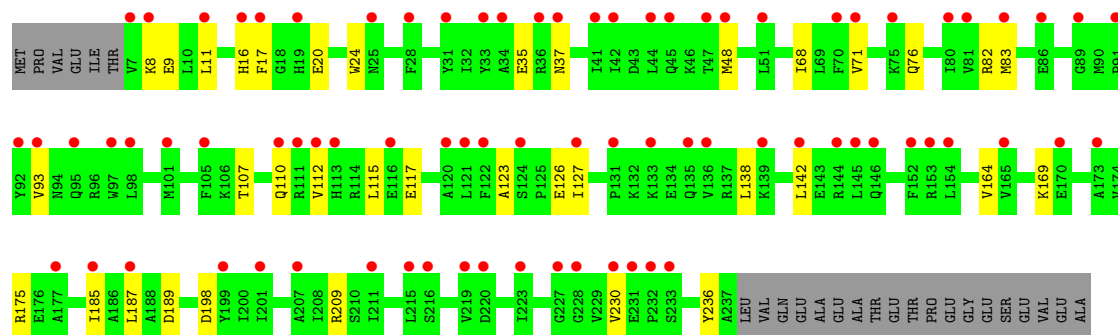
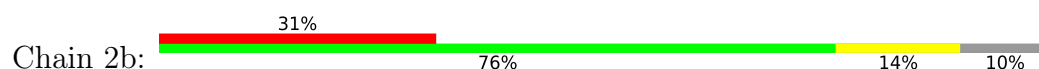




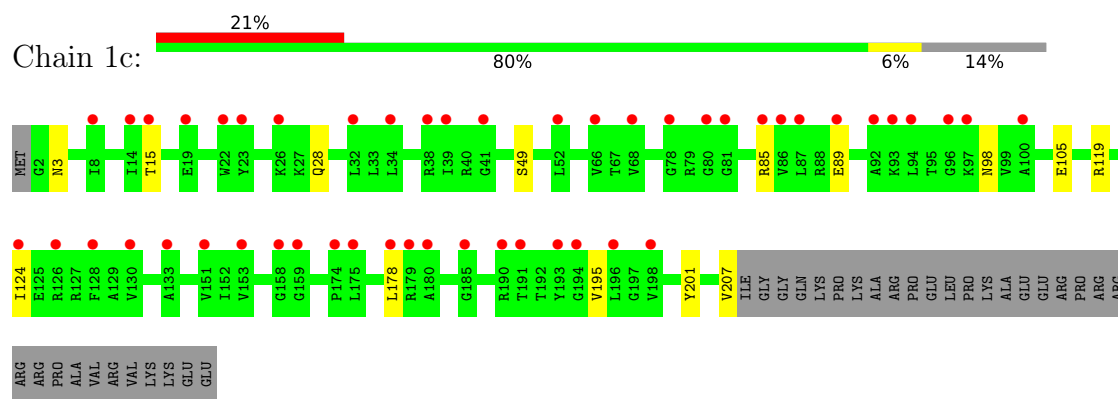
• Molecule 33: 30S ribosomal protein S2



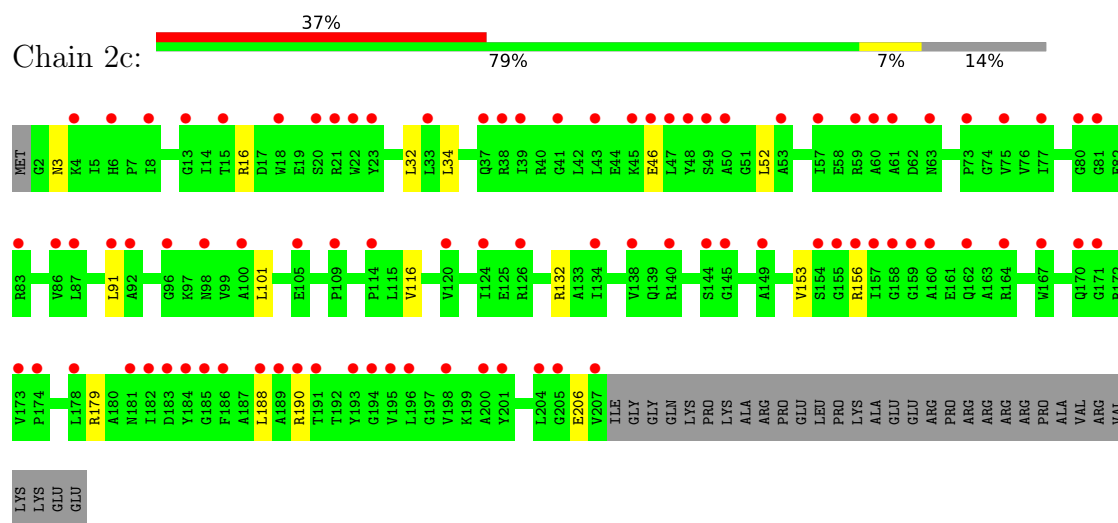
• Molecule 33: 30S ribosomal protein S2



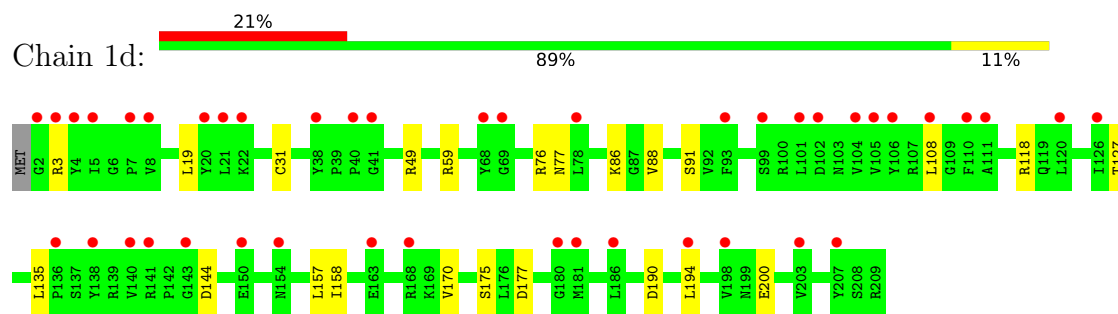
• Molecule 34: 30S ribosomal protein S3



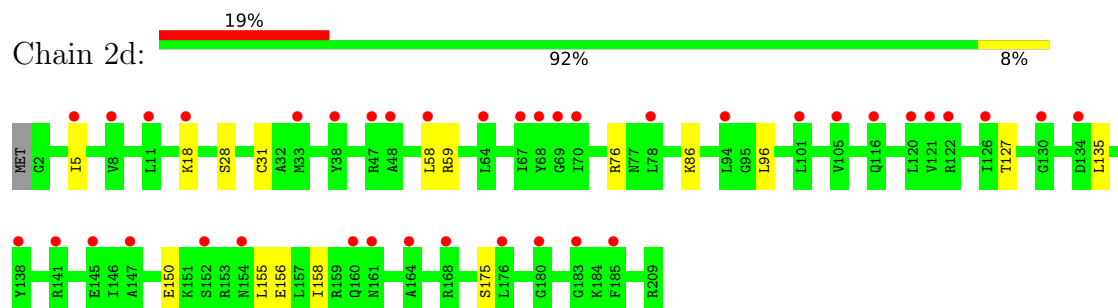
• Molecule 34: 30S ribosomal protein S3



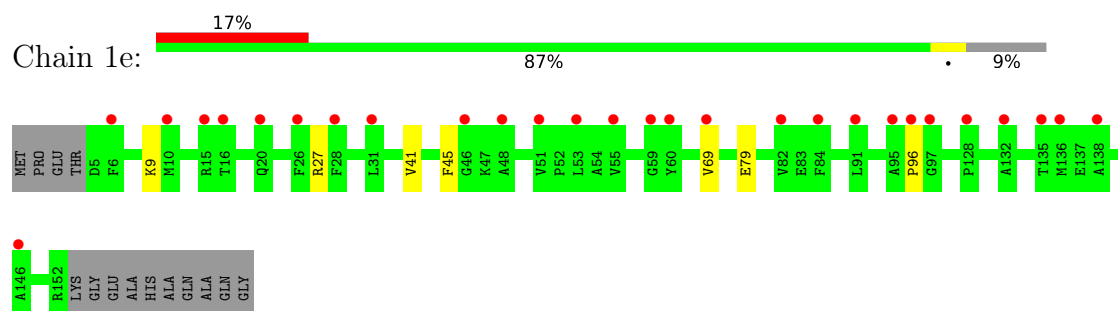
• Molecule 35: 30S ribosomal protein S4



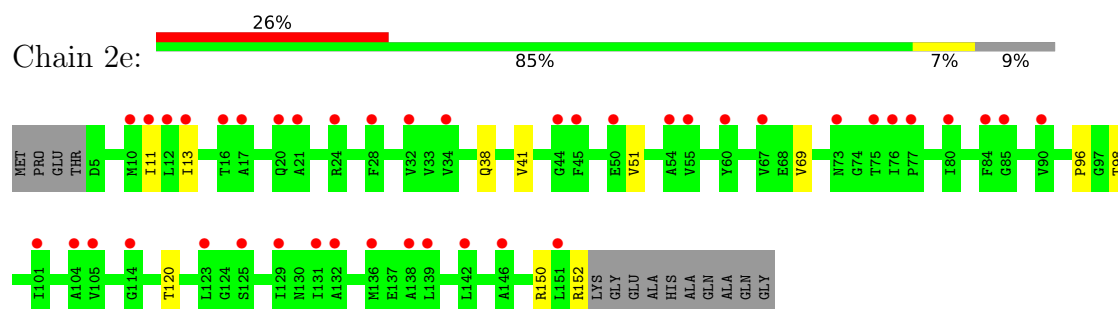
• Molecule 35: 30S ribosomal protein S4



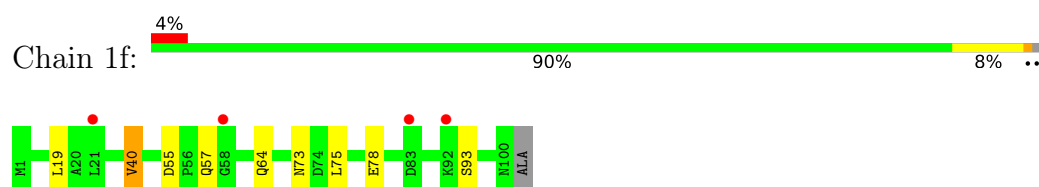
- Molecule 36: 30S ribosomal protein S5



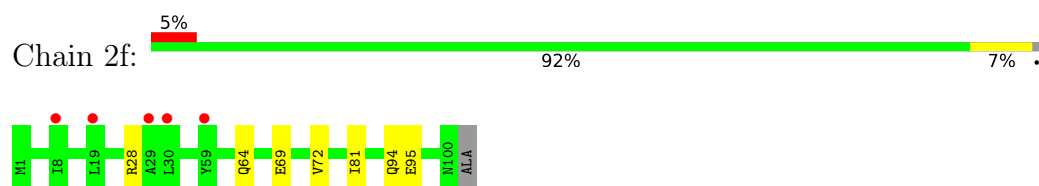
- Molecule 36: 30S ribosomal protein S5



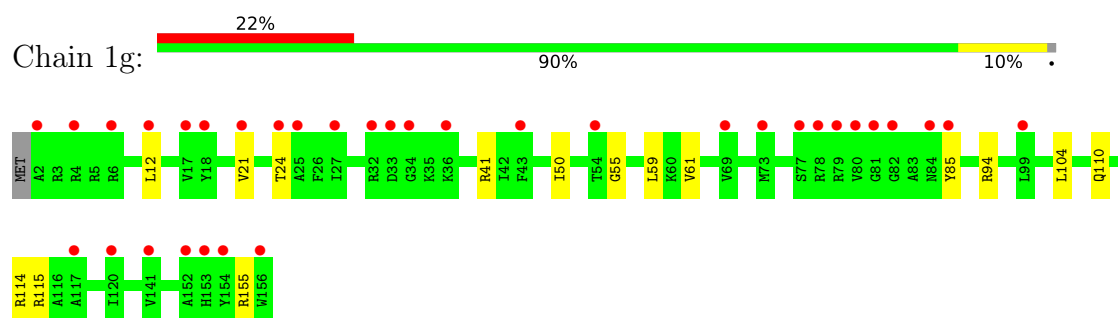
- Molecule 37: 30S ribosomal protein S6



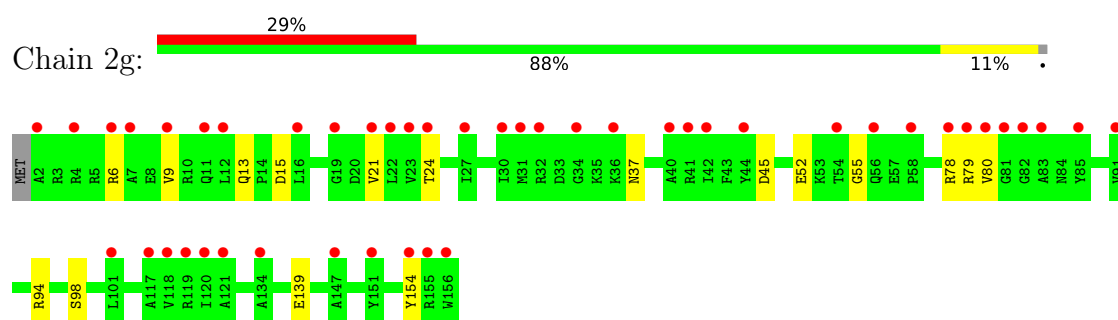
- Molecule 37: 30S ribosomal protein S6



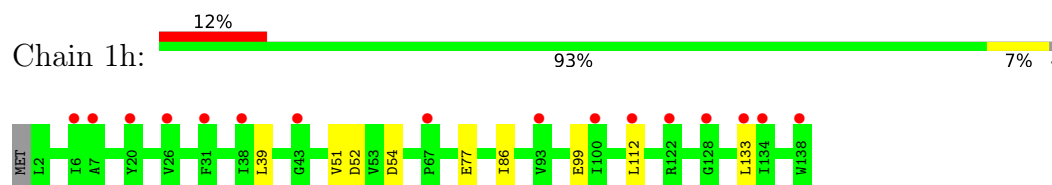
- Molecule 38: 30S ribosomal protein S7



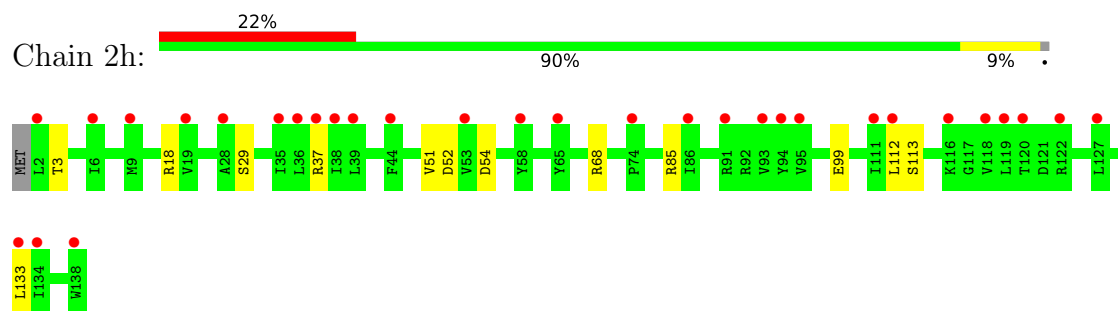
- Molecule 38: 30S ribosomal protein S7



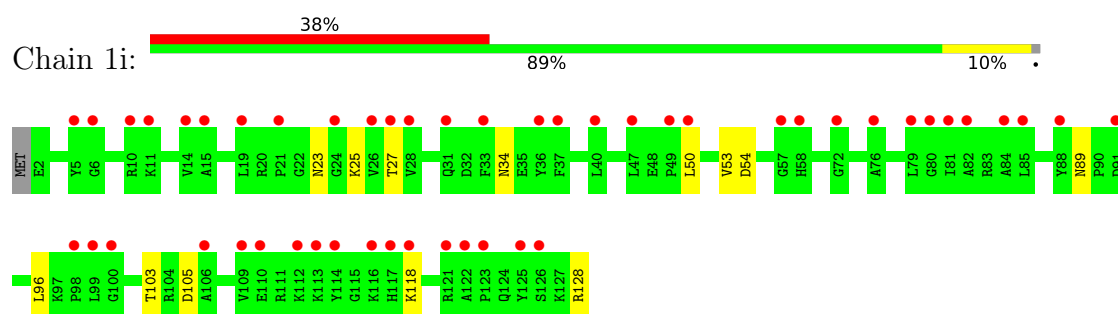
- Molecule 39: 30S ribosomal protein S8



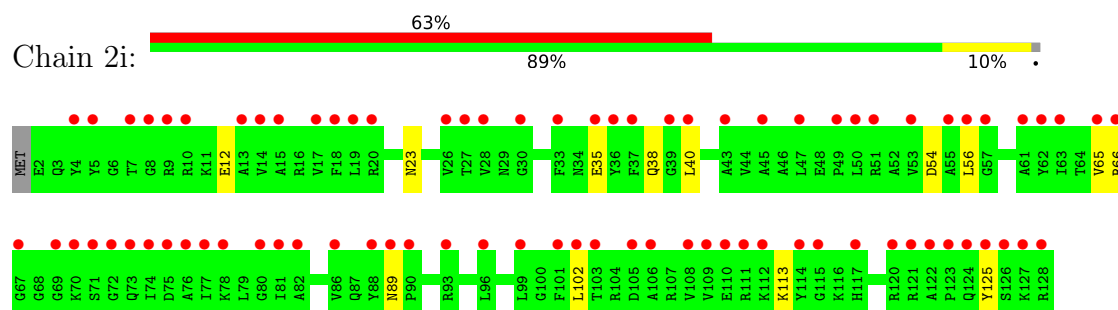
- Molecule 39: 30S ribosomal protein S8



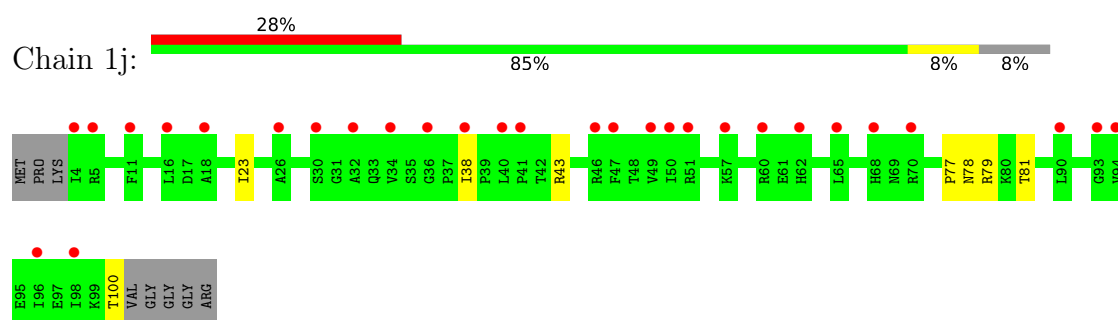
- Molecule 40: 30S ribosomal protein S9



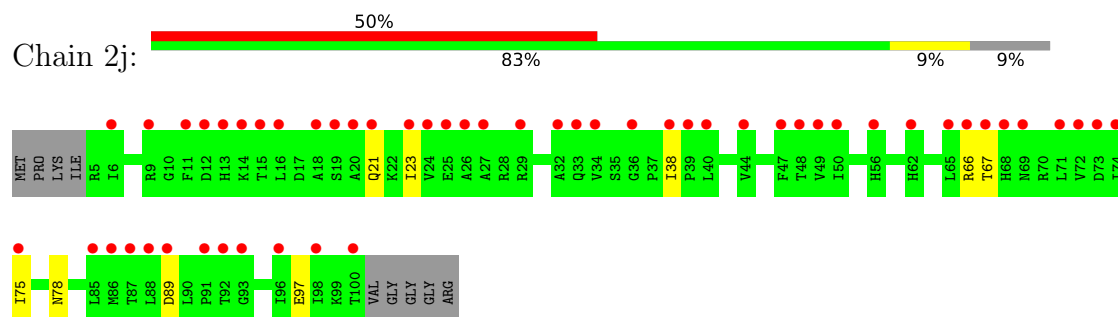
- Molecule 40: 30S ribosomal protein S9



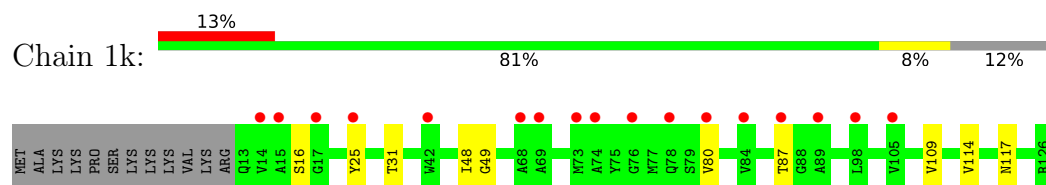
- Molecule 41: 30S ribosomal protein S10



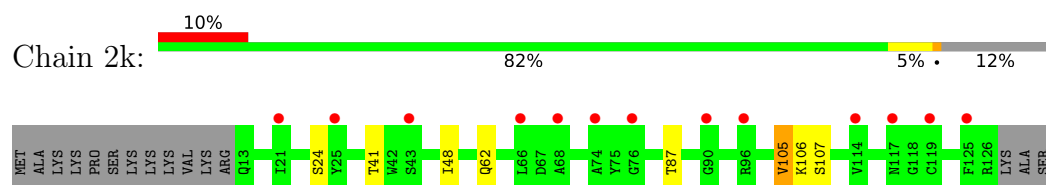
- Molecule 41: 30S ribosomal protein S10



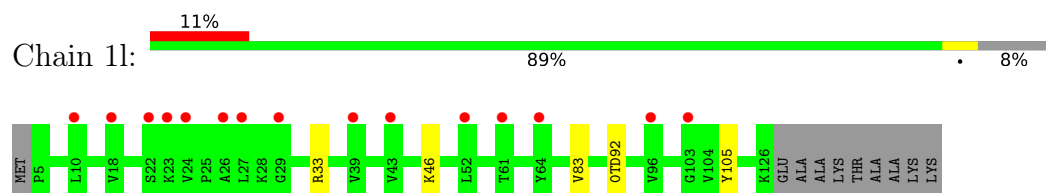
- Molecule 42: 30S ribosomal protein S11



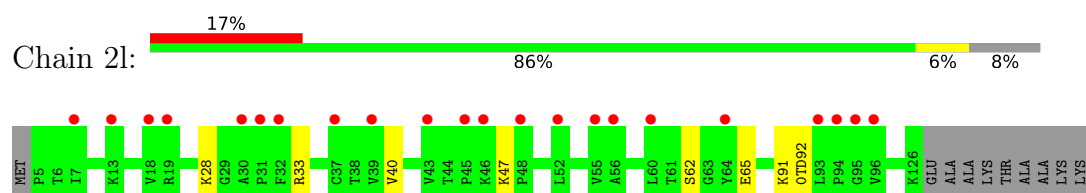
- Molecule 42: 30S ribosomal protein S11



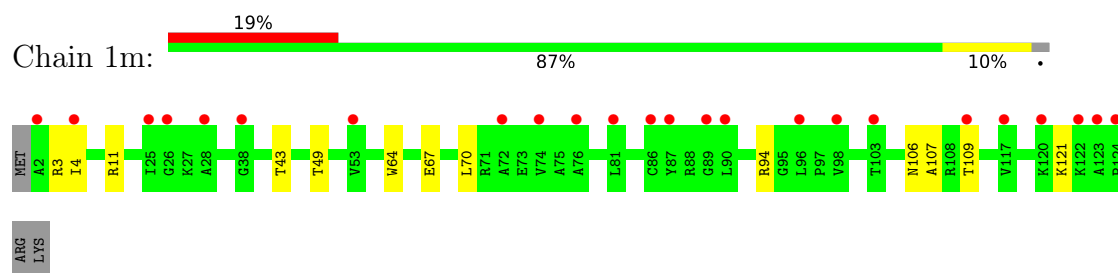
- Molecule 43: 30S ribosomal protein S12



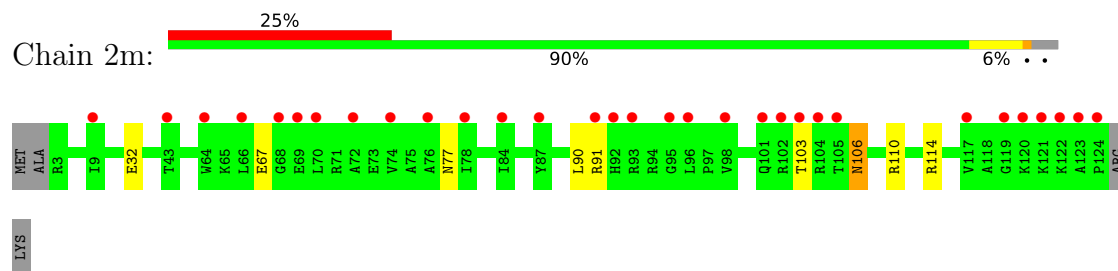
- Molecule 43: 30S ribosomal protein S12



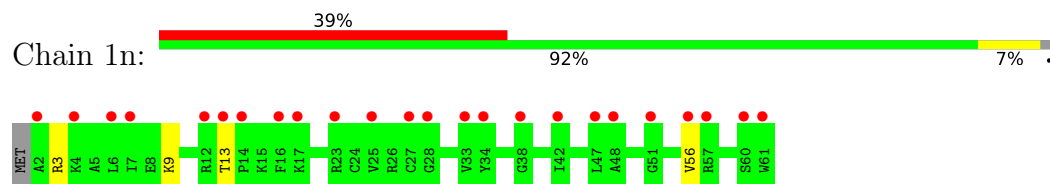
- Molecule 44: 30S ribosomal protein S13



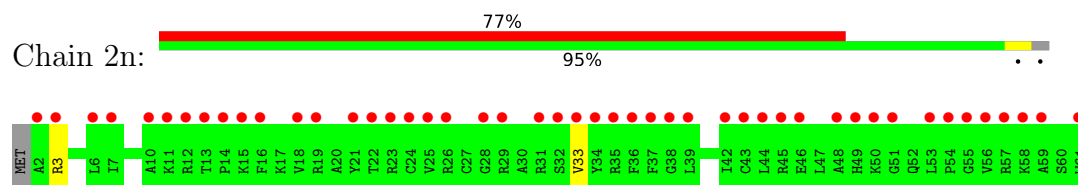
- Molecule 44: 30S ribosomal protein S13



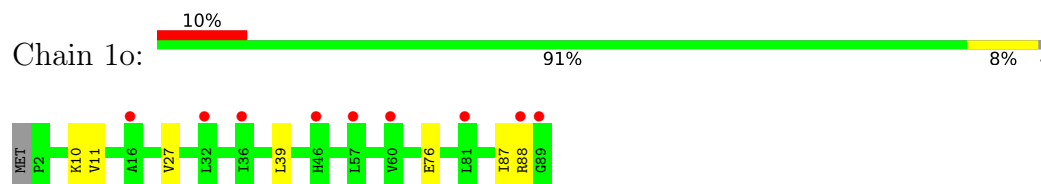
- Molecule 45: 30S ribosomal protein S14 type Z



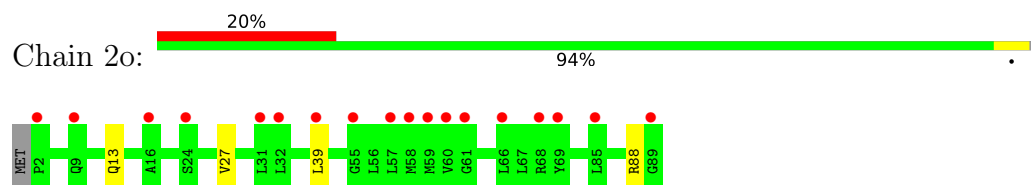
- Molecule 45: 30S ribosomal protein S14 type Z



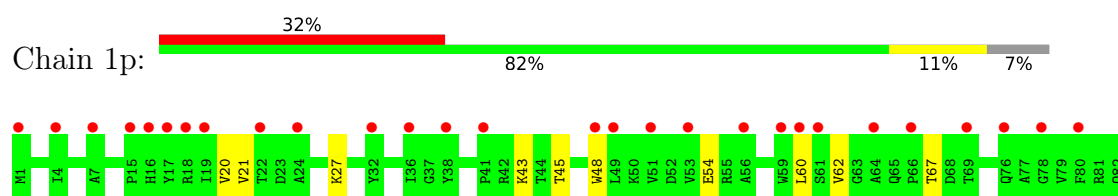
- Molecule 46: 30S ribosomal protein S15



- Molecule 46: 30S ribosomal protein S15

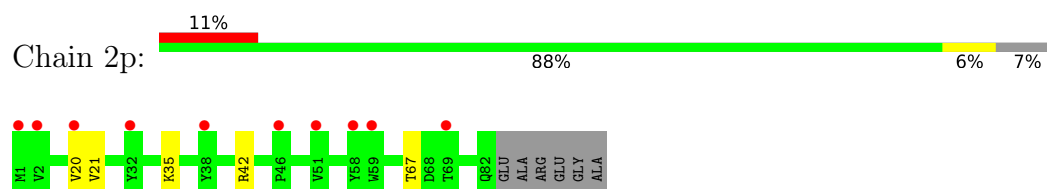


- Molecule 47: 30S ribosomal protein S16

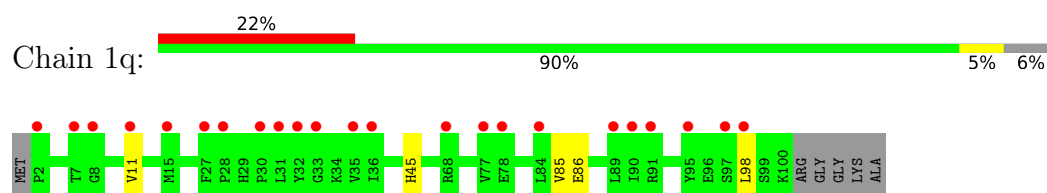


GLU
ALA
ARG
GLU
GLY
ALA

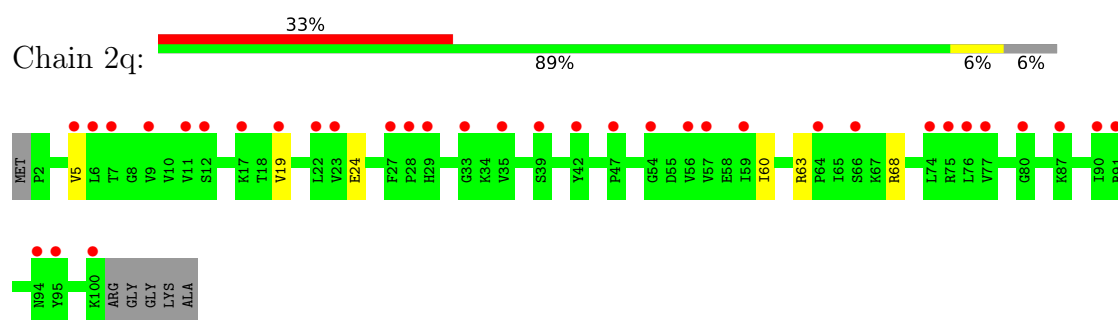
- Molecule 47: 30S ribosomal protein S16



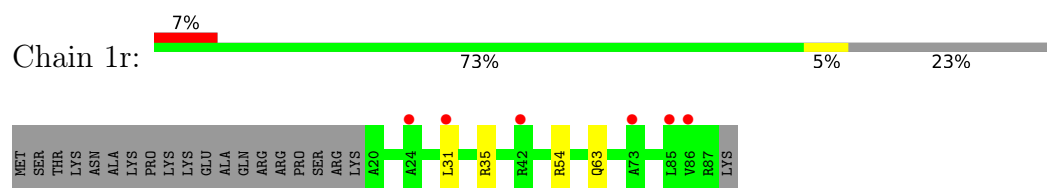
- Molecule 48: 30S ribosomal protein S17



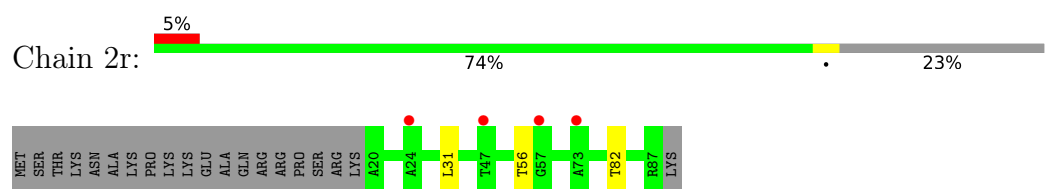
- Molecule 48: 30S ribosomal protein S17



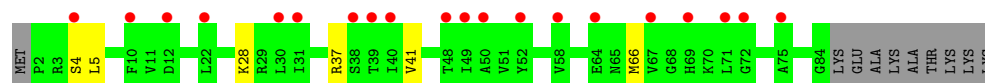
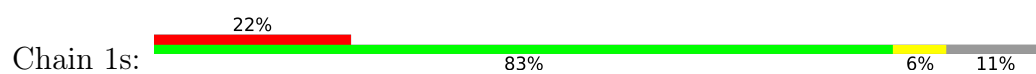
- Molecule 49: 30S ribosomal protein S18



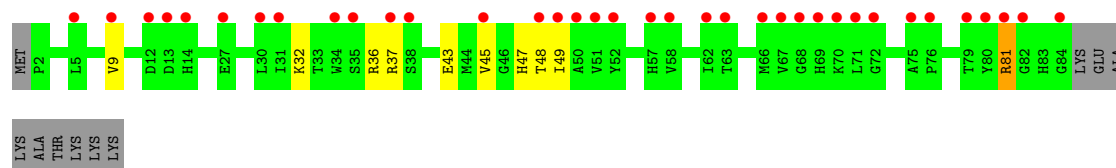
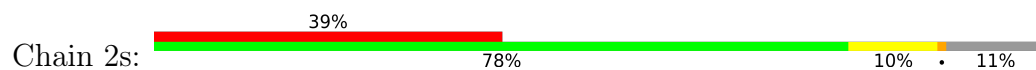
- Molecule 49: 30S ribosomal protein S18



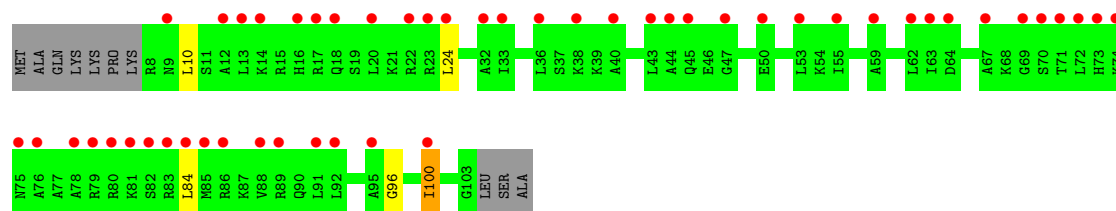
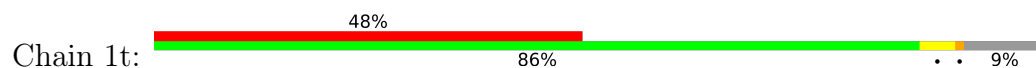
- Molecule 50: 30S ribosomal protein S19



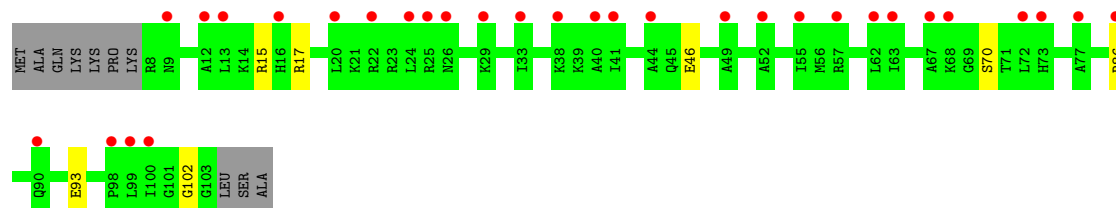
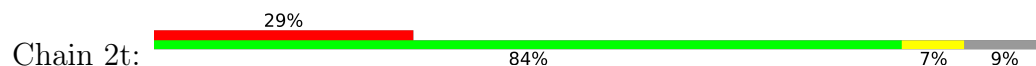
- Molecule 50: 30S ribosomal protein S19



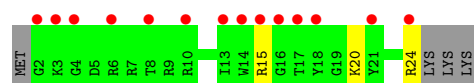
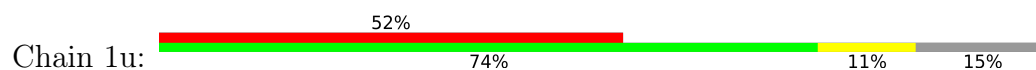
- Molecule 51: 30S ribosomal protein S20



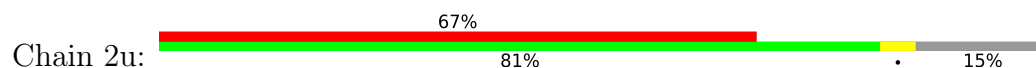
- Molecule 51: 30S ribosomal protein S20

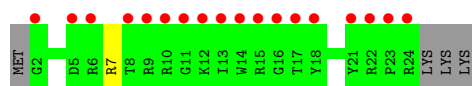


- Molecule 52: 30S ribosomal protein Thx



- Molecule 52: 30S ribosomal protein Thx

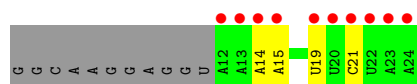
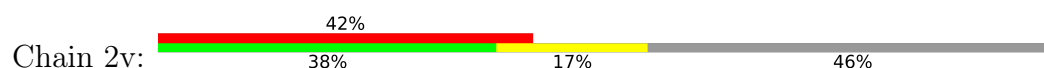




- Molecule 53: MF-mRNA



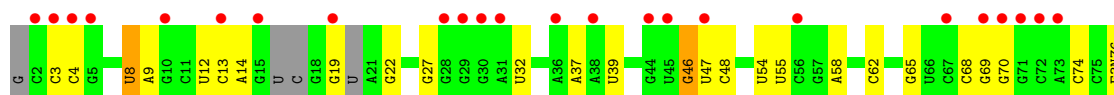
- Molecule 53: MF-mRNA



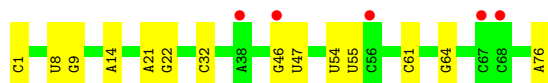
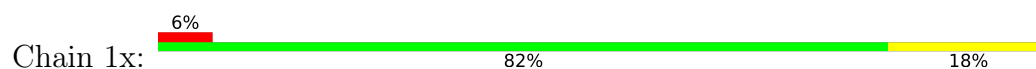
- Molecule 54: A-site Aminoacyl-tRNA Phe-NH-tRNAphe



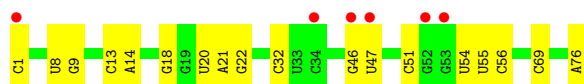
- Molecule 54: A-site Aminoacyl-tRNA Phe-NH-tRNAphe



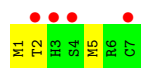
- Molecule 55: P-site Peptidyl-tRNA fMTHSMRC-NH-tRNAmet RNA-part



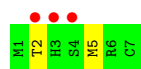
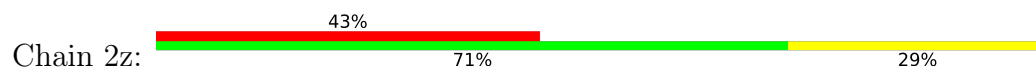
- Molecule 55: P-site Peptidyl-tRNA fMTHSMRC-NH-tRNAmet RNA-part



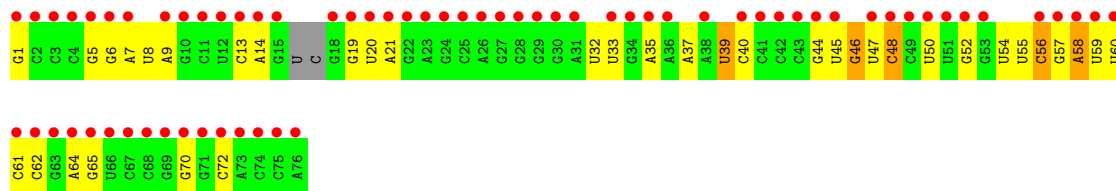
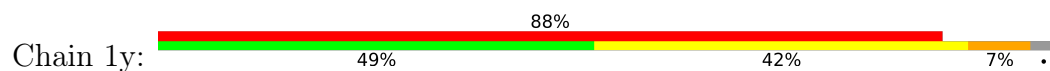
- Molecule 56: P-site Peptidyl-tRNA fMTHSMRC-NH-tRNAmet Peptide-part



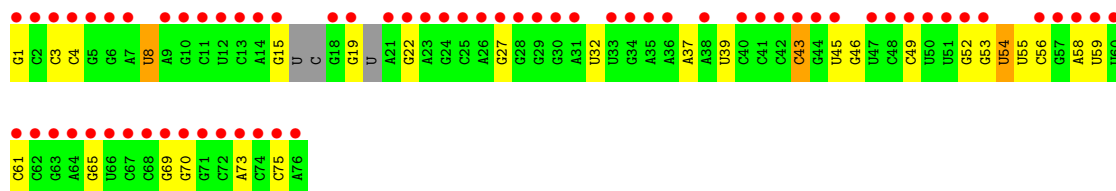
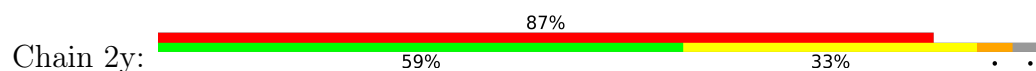
- Molecule 56: P-site Peptidyl-tRNA fMTHSMRC-NH-tRNA^{met} Peptide-part



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.43Å 447.70Å 618.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	121.53 – 2.30 181.36 – 2.47	Depositor EDS
% Data completeness (in resolution range)	97.5 (121.53-2.30) 98.6 (181.36-2.47)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.237 , 0.281 0.270 , 0.301	Depositor DCC
R_{free} test set	101013 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	41.7	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 48.4	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	0.87	EDS
Total number of atoms	299898	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 0TD, 5MU, MG, 8AN, SF4, 2MA, 4OC, PSU, OMU, 4SU, OMC, OMG, K, ZN, G7M, MA6, M2G, 2MG, FME, UR3, 5MC, MIA, F3N

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	0.50	0/69011	0.98	75/107720 (0.1%)
1	2A	0.39	0/67295	0.87	47/105042 (0.0%)
2	1B	0.45	1/2882 (0.0%)	0.89	0/4494
2	2B	0.38	1/2879 (0.0%)	0.83	2/4487 (0.0%)
3	1D	0.37	0/2186	0.56	0/2944
3	2D	0.32	0/2186	0.52	0/2944
4	1E	0.34	0/1592	0.55	0/2149
4	2E	0.29	0/1592	0.51	0/2149
5	1F	0.33	0/1618	0.54	0/2191
5	2F	0.30	0/1614	0.49	0/2186
6	1G	0.30	0/1448	0.50	0/1957
6	2G	0.28	0/1453	0.47	0/1963
7	1H	0.31	0/1356	0.50	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	0.29	0/1079	0.51	1/1475 (0.1%)
9	1N	0.32	0/1144	0.50	0/1543
9	2N	0.28	0/1144	0.45	0/1543
10	1O	0.34	0/943	0.56	0/1269
10	2O	0.30	0/943	0.55	0/1269
11	1P	0.33	0/1152	0.56	0/1533
11	2P	0.29	0/1152	0.52	0/1533
12	1Q	0.34	0/1143	0.53	0/1527
12	2Q	0.30	0/1143	0.48	0/1527
13	1R	0.32	0/982	0.53	0/1312
13	2R	0.27	0/982	0.49	0/1312
14	1S	0.32	0/883	0.51	0/1176
14	2S	0.29	0/880	0.48	0/1172
15	1T	0.31	0/1105	0.50	0/1477
15	2T	0.29	0/1097	0.49	0/1468
16	1U	0.34	0/977	0.53	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.30	0/977	0.44	0/1301
17	1V	0.33	0/782	0.57	0/1049
17	2V	0.29	0/782	0.51	0/1049
18	1W	0.35	0/897	0.53	0/1205
18	2W	0.30	0/897	0.49	0/1205
19	1X	0.35	0/764	0.55	0/1025
19	2X	0.29	0/764	0.55	0/1025
20	1Y	0.31	0/819	0.54	0/1095
20	2Y	0.28	0/819	0.47	0/1095
21	1Z	0.30	0/1267	0.51	0/1717
21	2Z	0.29	0/1299	0.51	0/1763
22	10	0.32	0/662	0.52	0/881
22	20	0.30	0/662	0.48	0/881
23	11	0.31	0/762	0.51	0/1014
23	21	0.30	0/762	0.50	0/1014
24	12	0.28	0/590	0.46	0/781
24	22	0.28	0/590	0.44	0/781
25	13	0.31	0/474	0.50	0/635
25	23	0.27	0/469	0.45	0/630
26	14	0.31	0/565	0.50	0/761
26	24	0.30	0/545	0.50	0/737
27	15	0.33	0/469	0.57	0/635
27	25	0.30	0/469	0.54	0/635
28	16	0.34	0/460	0.55	0/613
28	26	0.29	0/456	0.49	0/608
29	17	0.33	0/426	0.55	0/561
29	27	0.28	0/426	0.48	0/561
30	18	0.33	0/525	0.51	0/691
30	28	0.28	0/525	0.48	0/691
31	19	0.32	0/310	0.54	0/407
31	29	0.30	0/310	0.52	0/407
32	1a	0.36	0/35795	0.89	32/55864 (0.1%)
32	2a	0.34	2/35886 (0.0%)	0.89	38/56005 (0.1%)
33	1b	0.28	0/1881	0.48	0/2542
33	2b	0.30	0/1860	0.49	0/2518
34	1c	0.28	0/1572	0.48	0/2126
34	2c	0.27	0/1566	0.48	0/2119
35	1d	0.29	0/1685	0.49	0/2262
35	2d	0.28	0/1704	0.45	0/2284
36	1e	0.29	0/1145	0.52	0/1543
36	2e	0.29	0/1149	0.50	0/1548
37	1f	0.27	0/823	0.47	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	0.43	0/1679
38	2g	0.27	0/1254	0.43	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	0.51	0/1346
40	2i	0.29	0/997	0.53	0/1343
41	1j	0.27	0/722	0.49	0/982
41	2j	0.27	0/727	0.50	0/988
42	1k	0.28	0/844	0.47	0/1145
42	2k	0.28	0/848	0.46	0/1149
43	1l	0.30	0/937	0.50	0/1260
43	2l	0.28	0/937	0.50	0/1260
44	1m	0.29	0/969	0.52	0/1302
44	2m	0.27	0/961	0.47	0/1291
45	1n	0.31	0/501	0.50	0/664
45	2n	0.31	0/501	0.50	0/664
46	1o	0.27	0/739	0.40	0/985
46	2o	0.26	0/739	0.42	0/985
47	1p	0.27	0/697	0.50	0/939
47	2p	0.27	0/693	0.51	0/935
48	1q	0.29	0/836	0.48	0/1117
48	2q	0.27	0/836	0.47	0/1117
49	1r	0.28	0/560	0.49	0/746
49	2r	0.26	0/560	0.48	0/746
50	1s	0.30	0/667	0.51	0/900
50	2s	0.28	0/661	0.54	0/893
51	1t	0.27	0/730	0.46	0/965
51	2t	0.26	0/729	0.42	0/965
52	1u	0.27	0/203	0.50	0/266
52	2u	0.25	0/203	0.47	0/266
53	1v	0.43	0/310	0.92	0/480
53	2v	0.49	0/310	1.03	1/480 (0.2%)
54	1w	0.51	1/1581 (0.1%)	1.04	2/2458 (0.1%)
54	2w	0.42	0/1531	1.05	0/2379
55	1x	0.60	6/1723 (0.3%)	1.15	18/2684 (0.7%)
55	2x	0.54	2/1723 (0.1%)	1.10	15/2684 (0.6%)
56	1z	0.44	0/48	0.65	0/62
56	2z	0.38	0/48	0.57	0/62
57	1y	0.55	1/1606 (0.1%)	1.13	8/2497 (0.3%)
57	2y	0.55	1/1583 (0.1%)	1.08	4/2459 (0.2%)
All	All	0.39	15/316730 (0.0%)	0.83	244/474161 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
12	1Q	0	1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	1	G	OP3-P	-10.43	1.48	1.61
55	1x	1	C	OP3-P	-10.42	1.48	1.61
55	2x	1	C	OP3-P	-10.42	1.48	1.61
57	1y	1	G	OP3-P	-10.38	1.48	1.61
2	1B	1	U	OP3-P	-10.34	1.48	1.61
2	2B	1	U	OP3-P	-10.24	1.48	1.61
57	2y	1	G	OP3-P	-10.16	1.49	1.61
32	2a	1272	G	N1-C2	-8.13	1.31	1.37
32	2a	1272	G	C6-N1	-7.46	1.34	1.39
55	1x	22	G	N7-C5	7.22	1.43	1.39
55	2x	22	G	N7-C5	5.54	1.42	1.39
55	1x	46	G	C6-N1	5.43	1.43	1.39
55	1x	14	A	N9-C4	5.30	1.41	1.37
55	1x	14	A	C8-N7	-5.19	1.27	1.31
55	1x	14	A	N7-C5	-5.12	1.36	1.39

All (244) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1263	C	N1-C2-O2	22.43	132.36	118.90
32	2a	1272	G	N3-C2-N2	19.66	133.66	119.90
32	2a	1272	G	N1-C2-N2	-16.68	101.19	116.20
32	2a	1272	G	C5-C6-O6	16.43	138.46	128.60
32	2a	1263	C	C2-N3-C4	14.21	127.01	119.90
32	2a	1263	C	N3-C2-O2	-12.26	113.32	121.90
32	2a	1263	C	C5-C6-N1	12.00	127.00	121.00
1	2A	2136	C	N1-C2-O2	11.52	125.81	118.90
32	2a	1272	G	C6-N1-C2	11.51	132.00	125.10
55	1x	46	G	C6-N1-C2	-11.43	118.24	125.10
55	2x	46	G	C6-N1-C2	-11.03	118.48	125.10
1	1A	1075	C	N1-C2-O2	10.80	125.38	118.90
32	2a	1272	G	C5-C6-N1	-10.48	106.26	111.50
1	1A	512	G	O4'-C1'-N9	9.95	116.16	108.20
55	1x	14	A	C4-C5-C6	9.95	121.97	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2577	A	O5'-P-OP1	-9.64	97.03	105.70
1	1A	567	A	O5'-P-OP1	-9.53	97.12	105.70
1	1A	576	U	O5'-P-OP1	-9.50	97.15	105.70
1	1A	1063	G	C5-C6-O6	9.40	134.24	128.60
55	1x	14	A	C5-N7-C8	9.39	108.60	103.90
1	1A	1075	C	C2-N3-C4	9.39	124.60	119.90
32	1a	558	G	O5'-P-OP1	-9.31	97.32	105.70
1	2A	2155	G	C5-C6-O6	9.17	134.10	128.60
1	2A	2155	G	C6-N1-C2	8.95	130.47	125.10
32	2a	1263	C	C6-N1-C2	-8.89	116.74	120.30
32	2a	1263	C	C2-N1-C1'	8.88	128.57	118.80
55	2x	22	G	C5-N7-C8	-8.63	99.99	104.30
32	1a	254	G	O5'-P-OP1	-8.56	97.99	105.70
1	1A	1997	G	O5'-P-OP2	-8.49	98.06	105.70
55	1x	22	G	C5-N7-C8	-8.43	100.08	104.30
55	1x	22	G	N1-C6-O6	-8.36	114.89	119.90
32	2a	1272	G	C4-N9-C1'	8.29	137.28	126.50
55	2x	14	A	C5-N7-C8	8.29	108.05	103.90
1	2A	576	U	O5'-P-OP1	-8.25	98.27	105.70
55	1x	22	G	C4-C5-C6	-8.20	113.88	118.80
55	2x	46	G	N3-C2-N2	-8.18	114.17	119.90
57	1y	33	U	N3-C2-O2	-8.14	116.50	122.20
1	1A	1352	U	O5'-P-OP1	-8.12	98.39	105.70
1	1A	2573	C	N1-C2-O2	-8.08	114.05	118.90
57	1y	33	U	N1-C2-O2	8.02	128.41	122.80
55	2x	14	A	C4-C5-C6	7.94	120.97	117.00
1	1A	1086	A	N1-C6-N6	-7.93	113.84	118.60
32	2a	1263	C	C4-C5-C6	-7.91	113.45	117.40
2	2B	80	U	O4'-C1'-N1	7.90	114.52	108.20
1	1A	607	U	O5'-P-OP1	-7.87	98.62	105.70
1	1A	1063	G	C6-N1-C2	7.78	129.76	125.10
32	2a	1272	G	C8-N9-C1'	-7.77	116.90	127.00
55	1x	14	A	C5-C6-N1	-7.76	113.82	117.70
32	2a	1272	G	N1-C6-O6	-7.73	115.26	119.90
1	1A	1063	G	N3-C2-N2	7.72	125.31	119.90
1	1A	2036	C	O5'-P-OP1	-7.67	98.80	105.70
1	2A	1298	C	O5'-P-OP2	-7.50	98.95	105.70
1	1A	975	C	N1-C2-O2	-7.46	114.42	118.90
1	1A	999	U	O5'-P-OP2	-7.38	99.05	105.70
1	1A	787	U	O5'-P-OP1	-7.37	99.07	105.70
1	2A	2136	C	N3-C2-O2	-7.30	116.79	121.90
57	1y	33	U	C2-N1-C1'	7.22	126.37	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1272	G	C2-N3-C4	-7.20	108.30	111.90
1	2A	2136	C	C2-N3-C4	7.16	123.48	119.90
55	1x	22	G	C5-C6-N1	7.05	115.02	111.50
55	2x	22	G	C5-C6-N1	7.04	115.02	111.50
32	2a	1263	C	N1-C2-N3	-7.03	114.28	119.20
32	2a	1043	C	N1-C2-O2	6.98	123.09	118.90
1	1A	2593	U	N3-C4-O4	-6.97	114.52	119.40
32	1a	1034	G	C6-N1-C2	6.96	129.28	125.10
32	2a	754	C	C2-N1-C1'	6.96	126.45	118.80
32	2a	841	U	C5-C6-N1	6.89	126.15	122.70
55	1x	46	G	C5-C6-O6	-6.88	124.47	128.60
55	2x	22	G	C4-C5-C6	-6.86	114.69	118.80
32	2a	754	C	N1-C2-O2	6.76	122.96	118.90
1	1A	568	U	N3-C4-C5	6.75	118.65	114.60
1	2A	192	C	O5'-P-OP1	-6.75	99.63	105.70
1	2A	2492	U	O5'-P-OP1	-6.73	99.65	105.70
1	1A	2682	U	O5'-P-OP2	-6.66	99.70	105.70
1	1A	1776	G	O5'-P-OP2	-6.64	99.73	105.70
1	2A	2155	G	N3-C2-N2	6.60	124.52	119.90
32	1a	266	G	P-O3'-C3'	6.60	127.62	119.70
1	1A	2028	U	N3-C4-O4	-6.60	114.78	119.40
32	1a	1034	G	C5-C6-O6	6.58	132.55	128.60
32	1a	841	U	C2-N1-C1'	6.54	125.55	117.70
32	1a	1158	C	C2-N1-C1'	6.49	125.94	118.80
55	2x	14	A	C5-C6-N1	-6.47	114.46	117.70
55	1x	46	G	N1-C2-N3	6.45	127.77	123.90
57	1y	56	C	N1-C2-O2	6.41	122.75	118.90
1	1A	1249	U	O5'-P-OP1	-6.38	99.95	105.70
54	1w	47	U	C2-N1-C1'	6.35	125.32	117.70
1	1A	1614	A	O5'-P-OP1	-6.33	100.00	105.70
1	1A	1075	C	C5-C4-N4	6.32	124.62	120.20
32	2a	1158	C	C2-N1-C1'	6.28	125.71	118.80
55	2x	46	G	C5-C6-N1	6.27	114.63	111.50
55	1x	46	G	C5-C6-N1	6.25	114.62	111.50
1	1A	1992	G	P-O3'-C3'	6.24	127.19	119.70
1	1A	2554	U	O5'-P-OP1	-6.19	100.13	105.70
1	2A	801	G	O5'-P-OP2	-6.17	100.15	105.70
1	2A	2155	G	N1-C6-O6	-6.13	116.22	119.90
1	1A	1080	C	N1-C2-O2	6.13	122.58	118.90
32	1a	1029	C	C2-N3-C4	6.12	122.96	119.90
32	1a	1030(B)	C	N1-C2-O2	6.11	122.57	118.90
32	2a	754	C	N3-C2-O2	-6.06	117.66	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	943	U	O5'-P-OP2	-6.04	100.26	105.70
1	1A	746	A	O4'-C1'-N9	6.00	113.00	108.20
55	1x	22	G	C6-C5-N7	6.00	134.00	130.40
1	1A	527	C	N1-C2-O2	-6.00	115.30	118.90
32	2a	1054	C	C2-N1-C1'	6.00	125.40	118.80
1	2A	752	A	P-O3'-C3'	5.98	126.88	119.70
1	2A	1313	U	C2-N1-C1'	5.97	124.86	117.70
1	1A	1936	A	O4'-C1'-N9	5.96	112.97	108.20
57	1y	48	C	N1-C2-O2	-5.96	115.33	118.90
32	1a	754	C	C2-N1-C1'	5.95	125.35	118.80
32	2a	1065	U	P-O3'-C3'	5.95	126.84	119.70
55	1x	22	G	N3-C4-N9	-5.94	122.44	126.00
32	2a	1263	C	C5-C4-N4	5.93	124.35	120.20
1	2A	847	U	N3-C2-O2	-5.90	118.07	122.20
1	1A	1075	C	N3-C2-O2	-5.89	117.77	121.90
1	2A	1992	G	P-O3'-C3'	5.89	126.77	119.70
1	1A	1791	A	O5'-P-OP1	-5.87	100.42	105.70
1	2A	512	G	O4'-C1'-N9	5.86	112.89	108.20
1	2A	2689	U	N3-C2-O2	-5.85	118.11	122.20
1	1A	2689	U	P-O3'-C3'	5.82	126.69	119.70
32	1a	299	G	C4-C5-N7	5.82	113.13	110.80
1	2A	2615	U	O5'-P-OP1	-5.81	100.47	105.70
55	2x	46	G	N9-C4-C5	5.81	107.72	105.40
55	1x	14	A	C8-N9-C1'	-5.81	117.25	127.70
1	1A	819	A	O5'-P-OP1	-5.80	100.48	105.70
1	1A	372	G	O4'-C1'-N9	5.80	112.84	108.20
55	2x	46	G	N1-C2-N3	5.80	127.38	123.90
1	1A	250	G	C8-N9-C4	-5.76	104.09	106.40
1	2A	2689	U	P-O3'-C3'	5.75	126.60	119.70
1	1A	568	U	C5-C4-O4	-5.75	122.45	125.90
1	2A	1614	A	O5'-P-OP1	-5.75	100.53	105.70
55	1x	14	A	C4-N9-C1'	5.72	136.59	126.30
1	1A	1174	A	OP1-P-O3'	5.70	117.75	105.20
1	1A	2629	A	P-O3'-C3'	5.70	126.54	119.70
32	1a	1002	G	C4-N9-C1'	5.67	133.87	126.50
1	2A	847	U	C2-N1-C1'	5.65	124.48	117.70
55	1x	22	G	N7-C8-N9	5.65	115.92	113.10
1	2A	1698	A	O4'-C1'-N9	5.65	112.72	108.20
55	2x	22	G	C4-C5-N7	5.64	113.06	110.80
55	2x	46	G	C4-C5-N7	-5.63	108.55	110.80
32	2a	1158	C	N1-C2-O2	5.62	122.27	118.90
32	1a	1030(B)	C	C2-N1-C1'	5.61	124.97	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2167	U	C2-N1-C1'	5.61	124.43	117.70
2	2B	1	U	C2-N1-C1'	5.60	124.42	117.70
32	2a	204	U	C2-N1-C1'	5.60	124.42	117.70
1	2A	1664	A	O5'-P-OP2	-5.60	100.66	105.70
32	1a	1442	G	N3-C4-C5	-5.59	125.80	128.60
57	2y	43	C	C2-N1-C1'	5.58	124.94	118.80
1	1A	748	G	O4'-C1'-N9	5.57	112.65	108.20
1	1A	1190	G	C5-N7-C8	5.56	107.08	104.30
1	1A	1174	A	P-O3'-C3'	5.55	126.36	119.70
1	2A	2897	U	C2-N1-C1'	5.55	124.36	117.70
1	1A	2033	A	OP1-P-OP2	-5.55	111.28	119.60
32	1a	841	U	C5-C6-N1	5.54	125.47	122.70
32	1a	1030(B)	C	C6-N1-C2	-5.54	118.08	120.30
1	1A	2794	C	N1-C2-O2	5.54	122.22	118.90
1	1A	1080	C	C2-N3-C4	5.52	122.66	119.90
1	2A	1639	U	O5'-P-OP2	-5.49	100.76	105.70
1	1A	845	G	O4'-C1'-N9	5.49	112.59	108.20
1	1A	2249	U	N3-C4-O4	-5.47	115.57	119.40
1	1A	847	U	C2-N1-C1'	5.47	124.26	117.70
57	2y	22	G	N1-C6-O6	5.46	123.18	119.90
1	2A	228	A	OP1-P-O3'	5.46	117.21	105.20
55	2x	22	G	N7-C8-N9	5.46	115.83	113.10
1	1A	2685	G	N1-C6-O6	-5.45	116.63	119.90
32	1a	841	U	N1-C2-O2	5.44	126.61	122.80
1	1A	1082	U	N3-C4-O4	-5.43	115.60	119.40
1	2A	228	A	P-O3'-C3'	5.43	126.21	119.70
32	1a	1158	C	N1-C2-O2	5.42	122.15	118.90
1	2A	1313	U	O4'-C1'-N1	5.41	112.53	108.20
1	2A	847	U	N1-C2-O2	5.41	126.58	122.80
1	1A	1993	U	O5'-P-OP1	-5.39	100.85	105.70
1	1A	2848	G	O4'-C1'-N9	5.39	112.51	108.20
1	1A	1063	G	C5-C6-N1	-5.37	108.81	111.50
54	1w	47	U	N1-C2-O2	5.37	126.56	122.80
32	2a	1029	C	N1-C2-O2	5.37	122.12	118.90
1	2A	2712	U	O4'-C1'-N1	5.37	112.49	108.20
32	2a	266	G	P-O3'-C3'	5.36	126.13	119.70
1	1A	2497	A	N1-C6-N6	-5.36	115.39	118.60
1	2A	2136	C	N3-C4-C5	-5.35	119.76	121.90
32	1a	1029	C	N1-C2-O2	5.35	122.11	118.90
32	1a	1030(B)	C	N3-C2-O2	-5.34	118.16	121.90
55	1x	46	G	N9-C4-C5	5.34	107.54	105.40
32	2a	1065	U	OP2-P-O3'	5.33	116.92	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	2x	22	G	N1-C6-O6	-5.32	116.71	119.90
32	1a	1067	A	P-O3'-C3'	5.31	126.08	119.70
32	1a	90	U	N3-C2-O2	-5.30	118.49	122.20
32	2a	1263	C	N3-C4-N4	-5.30	114.29	118.00
1	1A	2015	A	OP2-P-O3'	5.28	116.82	105.20
7	2H	115	VAL	C-N-CA	-5.28	108.49	121.70
1	2A	2318	G	C4-N9-C1'	5.25	133.33	126.50
1	1A	674	G	C8-N9-C4	5.25	108.50	106.40
1	2A	746	A	O4'-C1'-N9	5.25	112.40	108.20
32	1a	1002	G	N3-C4-N9	5.25	129.15	126.00
1	2A	784	A	O4'-C1'-N9	5.24	112.39	108.20
32	1a	687	A	P-O3'-C3'	5.23	125.98	119.70
1	2A	1022	G	N3-C4-N9	-5.23	122.86	126.00
1	2A	1779	U	O4'-C1'-N1	5.23	112.39	108.20
1	1A	383	U	O4'-C1'-N1	5.22	112.38	108.20
57	1y	64	A	C5-C6-N6	5.22	127.88	123.70
1	1A	1847	A	O4'-C1'-N9	5.22	112.38	108.20
1	1A	784	A	OP1-P-O3'	5.21	116.66	105.20
1	1A	2500	U	C5-C4-O4	5.20	129.02	125.90
32	1a	975	A	O4'-C1'-N9	-5.20	104.04	108.20
1	1A	444	C	O5'-P-OP1	5.20	116.94	110.70
32	2a	1263	C	C6-N1-C1'	-5.19	114.57	120.80
1	2A	1313	U	N1-C2-O2	5.19	126.43	122.80
8	2I	58	LEU	CA-CB-CG	5.19	127.23	115.30
32	1a	299	G	C5-C6-O6	-5.19	125.49	128.60
1	1A	1190	G	C4-C5-N7	-5.18	108.73	110.80
1	1A	1660	C	O5'-P-OP2	-5.18	101.04	105.70
1	1A	2136	C	N1-C2-O2	5.18	122.01	118.90
1	2A	528	A	OP1-P-O3'	5.17	116.57	105.20
32	2a	687	A	P-O3'-C3'	5.16	125.89	119.70
32	1a	1002	G	N3-C4-C5	-5.15	126.03	128.60
1	1A	214	G	O4'-C1'-N9	5.15	112.32	108.20
1	2A	2155	G	N1-C2-N3	-5.14	120.82	123.90
1	2A	90	U	N3-C2-O2	-5.13	118.61	122.20
1	1A	198	C	O5'-P-OP2	-5.12	101.09	105.70
57	1y	56	C	C2-N3-C4	5.12	122.46	119.90
1	2A	265	A	O4'-C1'-N9	5.10	112.28	108.20
1	2A	1558	A	C2-N3-C4	-5.10	108.05	110.60
1	1A	740	U	O5'-P-OP2	-5.10	101.11	105.70
57	1y	58	A	P-O3'-C3'	5.09	125.81	119.70
32	1a	1225	A	C6-N1-C2	5.09	121.65	118.60
1	2A	9	U	C5-C6-N1	5.08	125.24	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1043	C	C2-N1-C1'	5.07	124.38	118.80
57	2y	4	C	C2-N3-C4	5.07	122.43	119.90
57	2y	3	C	N1-C2-O2	5.06	121.94	118.90
1	1A	2134	A	P-O3'-C3'	5.06	125.78	119.70
1	2A	784	A	OP1-P-O3'	5.06	116.34	105.20
1	1A	2586	C	C6-N1-C2	-5.06	118.28	120.30
32	1a	1225	A	C5-C6-N6	5.06	127.75	123.70
1	1A	1153	C	O5'-P-OP2	-5.05	101.16	105.70
1	1A	674	G	N9-C4-C5	-5.05	103.38	105.40
55	1x	46	G	N3-C4-C5	-5.04	126.08	128.60
1	2A	528	A	P-O3'-C3'	5.04	125.74	119.70
32	2a	841	U	C6-N1-C2	-5.03	117.98	121.00
32	1a	90	U	C2-N1-C1'	5.03	123.74	117.70
32	1a	952	U	C5-C4-O4	5.03	128.92	125.90
32	2a	913	A	P-O3'-C3'	5.02	125.73	119.70
32	2a	65	U	P-O3'-C3'	5.02	125.72	119.70
53	2v	21	C	O4'-C1'-N1	5.01	112.21	108.20
32	1a	1027	C	C6-N1-C1'	5.01	126.81	120.80
1	2A	2711	A	O5'-P-OP1	-5.01	101.19	105.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	1Q	15	GLY	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	256 (94%)	17 (6%)	0	100	100
3	2D	273/276 (99%)	258 (94%)	15 (6%)	0	100	100
4	1E	202/206 (98%)	190 (94%)	11 (5%)	1 (0%)	29	35
4	2E	202/206 (98%)	195 (96%)	6 (3%)	1 (0%)	29	35
5	1F	200/210 (95%)	195 (98%)	5 (2%)	0	100	100
5	2F	200/210 (95%)	187 (94%)	10 (5%)	3 (2%)	10	10
6	1G	179/182 (98%)	165 (92%)	14 (8%)	0	100	100
6	2G	179/182 (98%)	158 (88%)	19 (11%)	2 (1%)	14	15
7	1H	172/180 (96%)	165 (96%)	6 (4%)	1 (1%)	25	31
7	2H	172/180 (96%)	146 (85%)	24 (14%)	2 (1%)	13	14
8	1I	144/148 (97%)	128 (89%)	15 (10%)	1 (1%)	22	26
8	2I	144/148 (97%)	119 (83%)	23 (16%)	2 (1%)	11	11
9	1N	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
9	2N	138/140 (99%)	132 (96%)	5 (4%)	1 (1%)	22	26
10	1O	120/122 (98%)	112 (93%)	7 (6%)	1 (1%)	19	23
10	2O	120/122 (98%)	109 (91%)	10 (8%)	1 (1%)	19	23
11	1P	147/150 (98%)	136 (92%)	10 (7%)	1 (1%)	22	26
11	2P	147/150 (98%)	127 (86%)	15 (10%)	5 (3%)	3	2
12	1Q	139/141 (99%)	132 (95%)	7 (5%)	0	100	100
12	2Q	139/141 (99%)	129 (93%)	10 (7%)	0	100	100
13	1R	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
13	2R	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
14	1S	108/112 (96%)	104 (96%)	4 (4%)	0	100	100
14	2S	108/112 (96%)	103 (95%)	3 (3%)	2 (2%)	8	7
15	1T	129/146 (88%)	121 (94%)	8 (6%)	0	100	100
15	2T	129/146 (88%)	121 (94%)	8 (6%)	0	100	100
16	1U	114/118 (97%)	114 (100%)	0	0	100	100
16	2U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
17	1V	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	15	17
17	2V	99/101 (98%)	92 (93%)	6 (6%)	1 (1%)	15	17
18	1W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
18	2W	110/113 (97%)	108 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	1X	93/96 (97%)	90 (97%)	2 (2%)	1 (1%)	14	15
19	2X	93/96 (97%)	87 (94%)	6 (6%)	0	100	100
20	1Y	105/110 (96%)	97 (92%)	8 (8%)	0	100	100
20	2Y	105/110 (96%)	100 (95%)	5 (5%)	0	100	100
21	1Z	148/206 (72%)	131 (88%)	16 (11%)	1 (1%)	22	26
21	2Z	156/206 (76%)	128 (82%)	23 (15%)	5 (3%)	4	2
22	10	81/85 (95%)	79 (98%)	2 (2%)	0	100	100
22	20	81/85 (95%)	77 (95%)	4 (5%)	0	100	100
23	11	95/98 (97%)	93 (98%)	2 (2%)	0	100	100
23	21	95/98 (97%)	90 (95%)	4 (4%)	1 (1%)	14	15
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	66 (97%)	1 (2%)	1 (2%)	10	10
25	13	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
25	23	57/60 (95%)	53 (93%)	3 (5%)	1 (2%)	8	7
26	14	67/71 (94%)	53 (79%)	10 (15%)	4 (6%)	1	0
26	24	67/71 (94%)	51 (76%)	14 (21%)	2 (3%)	4	2
27	15	57/60 (95%)	57 (100%)	0	0	100	100
27	25	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
28	16	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
28	26	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
29	17	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
29	27	46/49 (94%)	46 (100%)	0	0	100	100
30	18	62/65 (95%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	62 (100%)	0	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	35 (100%)	0	0	100	100
33	1b	229/256 (90%)	196 (86%)	27 (12%)	6 (3%)	5	4
33	2b	229/256 (90%)	196 (86%)	29 (13%)	4 (2%)	9	8
34	1c	204/239 (85%)	190 (93%)	14 (7%)	0	100	100
34	2c	204/239 (85%)	180 (88%)	22 (11%)	2 (1%)	15	17
35	1d	206/209 (99%)	190 (92%)	16 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	2d	206/209 (99%)	188 (91%)	18 (9%)	0	100	100
36	1e	146/162 (90%)	134 (92%)	10 (7%)	2 (1%)	11	11
36	2e	146/162 (90%)	130 (89%)	12 (8%)	4 (3%)	5	3
37	1f	98/101 (97%)	95 (97%)	2 (2%)	1 (1%)	15	17
37	2f	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
38	1g	153/156 (98%)	139 (91%)	13 (8%)	1 (1%)	22	26
38	2g	153/156 (98%)	133 (87%)	17 (11%)	3 (2%)	7	6
39	1h	135/138 (98%)	129 (96%)	6 (4%)	0	100	100
39	2h	135/138 (98%)	127 (94%)	8 (6%)	0	100	100
40	1i	125/128 (98%)	107 (86%)	17 (14%)	1 (1%)	19	23
40	2i	125/128 (98%)	106 (85%)	18 (14%)	1 (1%)	19	23
41	1j	95/105 (90%)	84 (88%)	8 (8%)	3 (3%)	4	2
41	2j	94/105 (90%)	77 (82%)	15 (16%)	2 (2%)	7	5
42	1k	112/129 (87%)	100 (89%)	11 (10%)	1 (1%)	17	20
42	2k	112/129 (87%)	100 (89%)	10 (9%)	2 (2%)	8	7
43	1l	119/132 (90%)	109 (92%)	9 (8%)	1 (1%)	19	23
43	2l	119/132 (90%)	109 (92%)	9 (8%)	1 (1%)	19	23
44	1m	121/126 (96%)	102 (84%)	17 (14%)	2 (2%)	9	8
44	2m	120/126 (95%)	104 (87%)	14 (12%)	2 (2%)	9	8
45	1n	58/61 (95%)	54 (93%)	4 (7%)	0	100	100
45	2n	58/61 (95%)	53 (91%)	5 (9%)	0	100	100
46	1o	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
46	2o	86/89 (97%)	79 (92%)	6 (7%)	1 (1%)	13	14
47	1p	80/88 (91%)	76 (95%)	4 (5%)	0	100	100
47	2p	80/88 (91%)	70 (88%)	10 (12%)	0	100	100
48	1q	97/105 (92%)	89 (92%)	8 (8%)	0	100	100
48	2q	97/105 (92%)	86 (89%)	10 (10%)	1 (1%)	15	17
49	1r	66/88 (75%)	61 (92%)	5 (8%)	0	100	100
49	2r	66/88 (75%)	64 (97%)	2 (3%)	0	100	100
50	1s	81/93 (87%)	72 (89%)	9 (11%)	0	100	100
50	2s	81/93 (87%)	65 (80%)	14 (17%)	2 (2%)	5	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	1t	94/106 (89%)	83 (88%)	9 (10%)	2 (2%)	7	5
51	2t	94/106 (89%)	84 (89%)	9 (10%)	1 (1%)	14	15
52	1u	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
52	2u	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
56	1z	5/7 (71%)	4 (80%)	0	1 (20%)	0	0
56	2z	5/7 (71%)	4 (80%)	0	1 (20%)	0	0
All	All	11378/12142 (94%)	10471 (92%)	817 (7%)	90 (1%)	19	23

All (90) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
21	1Z	53	ILE
26	14	47	GLN
26	14	62	ARG
33	1b	17	PHE
33	1b	124	SER
42	1k	49	GLY
44	1m	67	GLU
44	1m	107	ALA
56	1z	2	THR
5	2F	130	ALA
33	2b	17	PHE
33	2b	20	GLU
33	2b	123	ALA
33	2b	126	GLU
34	2c	179	ARG
38	2g	80	VAL
8	1I	11	ASN
19	1X	93	GLU
26	14	53	GLU
33	1b	126	GLU
40	1i	54	ASP
51	1t	96	GLY
6	2G	42	GLY
6	2G	43	LEU
8	2I	10	GLU
11	2P	38	GLN
21	2Z	146	ILE
23	21	3	LYS
26	24	45	GLY

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Mol	Chain	Res	Type
38	2g	55	GLY
41	2j	75	ILE
44	2m	67	GLU
44	2m	106	ASN
46	2o	88	ARG
48	2q	68	ARG
50	2s	9	VAL
50	2s	81	ARG
4	1E	52	LEU
7	1H	126	PRO
26	14	49	PHE
33	1b	8	LYS
41	1j	78	ASN
7	2H	126	PRO
10	2O	29	ASN
14	2S	84	GLN
21	2Z	93	ASP
36	2e	98	THR
42	2k	106	LYS
56	2z	2	THR
17	1V	79	VAL
33	1b	125	PRO
41	1j	77	PRO
41	1j	79	ARG
43	1l	105	TYR
4	2E	52	LEU
5	2F	18	ARG
5	2F	21	ALA
8	2I	41	GLU
9	2N	2	LYS
11	2P	29	LYS
11	2P	36	LYS
11	2P	45	LEU
21	2Z	52	SER
24	22	43	GLN
26	24	47	GLN
36	2e	69	VAL
43	2l	91	LYS
10	1O	5	GLN
11	1P	45	LEU
14	2S	96	GLY
17	2V	79	VAL

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Mol	Chain	Res	Type
36	2e	11	ILE
38	2g	52	GLU
40	2i	56	LEU
41	2j	78	ASN
33	1b	231	GLU
36	1e	69	VAL
36	1e	96	PRO
38	1g	55	GLY
11	2P	122	PRO
21	2Z	144	LEU
34	2c	156	ARG
21	2Z	167	PRO
7	2H	92	ILE
36	2e	96	PRO
51	1t	100	ILE
51	2t	102	GLY
37	1f	40	VAL
25	23	59	VAL
42	2k	105	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%)	206 (96%)	9 (4%)	30	42
3	2D	215/218 (99%)	205 (95%)	10 (5%)	26	37
4	1E	164/166 (99%)	154 (94%)	10 (6%)	18	25
4	2E	164/166 (99%)	153 (93%)	11 (7%)	16	21
5	1F	160/166 (96%)	146 (91%)	14 (9%)	10	12
5	2F	159/166 (96%)	149 (94%)	10 (6%)	18	24
6	1G	143/156 (92%)	129 (90%)	14 (10%)	8	9
6	2G	143/156 (92%)	124 (87%)	19 (13%)	4	4
7	1H	144/148 (97%)	137 (95%)	7 (5%)	25	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	2H	144/148 (97%)	135 (94%)	9 (6%)	18	24
8	1I	113/124 (91%)	95 (84%)	18 (16%)	2	2
8	2I	105/124 (85%)	85 (81%)	20 (19%)	1	1
9	1N	118/119 (99%)	110 (93%)	8 (7%)	16	21
9	2N	118/119 (99%)	111 (94%)	7 (6%)	19	27
10	1O	100/100 (100%)	97 (97%)	3 (3%)	41	57
10	2O	100/100 (100%)	98 (98%)	2 (2%)	55	72
11	1P	115/116 (99%)	107 (93%)	8 (7%)	15	19
11	2P	115/116 (99%)	103 (90%)	12 (10%)	7	8
12	1Q	111/111 (100%)	105 (95%)	6 (5%)	22	30
12	2Q	111/111 (100%)	109 (98%)	2 (2%)	59	75
13	1R	101/101 (100%)	94 (93%)	7 (7%)	15	20
13	2R	101/101 (100%)	94 (93%)	7 (7%)	15	20
14	1S	86/88 (98%)	82 (95%)	4 (5%)	26	37
14	2S	85/88 (97%)	77 (91%)	8 (9%)	8	10
15	1T	115/127 (91%)	110 (96%)	5 (4%)	29	40
15	2T	113/127 (89%)	104 (92%)	9 (8%)	12	15
16	1U	93/94 (99%)	90 (97%)	3 (3%)	39	54
16	2U	93/94 (99%)	88 (95%)	5 (5%)	22	30
17	1V	80/82 (98%)	74 (92%)	6 (8%)	13	17
17	2V	80/82 (98%)	72 (90%)	8 (10%)	7	9
18	1W	90/92 (98%)	84 (93%)	6 (7%)	16	21
18	2W	90/92 (98%)	83 (92%)	7 (8%)	12	16
19	1X	77/78 (99%)	75 (97%)	2 (3%)	46	63
19	2X	77/78 (99%)	74 (96%)	3 (4%)	32	46
20	1Y	85/91 (93%)	79 (93%)	6 (7%)	14	19
20	2Y	85/91 (93%)	72 (85%)	13 (15%)	2	2
21	1Z	135/179 (75%)	124 (92%)	11 (8%)	11	15
21	2Z	137/179 (76%)	117 (85%)	20 (15%)	3	3
22	10	65/67 (97%)	65 (100%)	0	100	100
22	20	65/67 (97%)	64 (98%)	1 (2%)	65	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	11	80/83 (96%)	77 (96%)	3 (4%)	33	47
23	21	80/83 (96%)	75 (94%)	5 (6%)	18	24
24	12	65/67 (97%)	60 (92%)	5 (8%)	13	16
24	22	65/67 (97%)	61 (94%)	4 (6%)	18	25
25	13	51/52 (98%)	48 (94%)	3 (6%)	19	27
25	23	50/52 (96%)	46 (92%)	4 (8%)	12	15
26	14	59/63 (94%)	51 (86%)	8 (14%)	3	3
26	24	53/63 (84%)	47 (89%)	6 (11%)	6	6
27	15	50/52 (96%)	46 (92%)	4 (8%)	12	15
27	25	50/52 (96%)	47 (94%)	3 (6%)	19	26
28	16	51/52 (98%)	46 (90%)	5 (10%)	8	9
28	26	50/52 (96%)	43 (86%)	7 (14%)	3	3
29	17	41/42 (98%)	38 (93%)	3 (7%)	14	18
29	27	41/42 (98%)	37 (90%)	4 (10%)	8	9
30	18	54/55 (98%)	51 (94%)	3 (6%)	21	29
30	28	54/55 (98%)	51 (94%)	3 (6%)	21	29
31	19	34/34 (100%)	33 (97%)	1 (3%)	42	58
31	29	34/34 (100%)	34 (100%)	0	100	100
33	1b	192/220 (87%)	167 (87%)	25 (13%)	4	4
33	2b	187/220 (85%)	155 (83%)	32 (17%)	2	2
34	1c	142/188 (76%)	128 (90%)	14 (10%)	8	9
34	2c	140/188 (74%)	126 (90%)	14 (10%)	7	9
35	1d	169/181 (93%)	146 (86%)	23 (14%)	3	3
35	2d	173/181 (96%)	157 (91%)	16 (9%)	9	11
36	1e	113/123 (92%)	108 (96%)	5 (4%)	28	39
36	2e	114/123 (93%)	107 (94%)	7 (6%)	18	25
37	1f	84/90 (93%)	75 (89%)	9 (11%)	6	7
37	2f	85/90 (94%)	78 (92%)	7 (8%)	11	14
38	1g	119/127 (94%)	105 (88%)	14 (12%)	5	5
38	2g	120/127 (94%)	106 (88%)	14 (12%)	5	6
39	1h	114/119 (96%)	105 (92%)	9 (8%)	12	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	2h	114/119 (96%)	101 (89%)	13 (11%)	5	6
40	1i	90/99 (91%)	78 (87%)	12 (13%)	4	4
40	2i	89/99 (90%)	77 (86%)	12 (14%)	4	4
41	1j	66/92 (72%)	61 (92%)	5 (8%)	13	16
41	2j	69/92 (75%)	62 (90%)	7 (10%)	7	9
42	1k	82/99 (83%)	73 (89%)	9 (11%)	6	7
42	2k	83/99 (84%)	76 (92%)	7 (8%)	11	13
43	1l	96/108 (89%)	93 (97%)	3 (3%)	40	55
43	2l	96/108 (89%)	90 (94%)	6 (6%)	18	24
44	1m	93/101 (92%)	82 (88%)	11 (12%)	5	5
44	2m	92/101 (91%)	84 (91%)	8 (9%)	10	12
45	1n	49/50 (98%)	45 (92%)	4 (8%)	11	14
45	2n	49/50 (98%)	47 (96%)	2 (4%)	30	43
46	1o	78/80 (98%)	71 (91%)	7 (9%)	9	11
46	2o	78/80 (98%)	75 (96%)	3 (4%)	33	47
47	1p	69/74 (93%)	59 (86%)	10 (14%)	3	3
47	2p	68/74 (92%)	63 (93%)	5 (7%)	13	17
48	1q	94/97 (97%)	89 (95%)	5 (5%)	22	31
48	2q	94/97 (97%)	89 (95%)	5 (5%)	22	31
49	1r	59/77 (77%)	55 (93%)	4 (7%)	16	21
49	2r	59/77 (77%)	56 (95%)	3 (5%)	24	33
50	1s	69/80 (86%)	63 (91%)	6 (9%)	10	12
50	2s	67/80 (84%)	58 (87%)	9 (13%)	4	4
51	1t	70/82 (85%)	66 (94%)	4 (6%)	20	28
51	2t	70/82 (85%)	64 (91%)	6 (9%)	10	12
52	1u	18/22 (82%)	15 (83%)	3 (17%)	2	2
52	2u	18/22 (82%)	17 (94%)	1 (6%)	21	29
56	1z	6/6 (100%)	5 (83%)	1 (17%)	2	2
56	2z	6/6 (100%)	5 (83%)	1 (17%)	2	2
All	All	9315/10076 (92%)	8553 (92%)	762 (8%)	11	14

All (762) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	14	ARG
3	1D	38	LYS
3	1D	99	ASP
3	1D	142	VAL
3	1D	154	LYS
3	1D	229	VAL
3	1D	242	ARG
3	1D	259	THR
3	1D	273	ARG
4	1E	12	THR
4	1E	47	VAL
4	1E	55	ASN
4	1E	87	GLU
4	1E	89	ASP
4	1E	90	THR
4	1E	93	VAL
4	1E	113	PHE
4	1E	116	VAL
4	1E	184	VAL
5	1F	24	LEU
5	1F	33	LEU
5	1F	53	THR
5	1F	57	VAL
5	1F	70	THR
5	1F	88	VAL
5	1F	106	ARG
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	192	LEU
6	1G	3	LEU
6	1G	5	VAL
6	1G	7	LEU
6	1G	21	ARG
6	1G	22	ARG
6	1G	31	VAL
6	1G	35	GLU
6	1G	36	LYS
6	1G	43	LEU
6	1G	91	ARG

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Mol	Chain	Res	Type
6	1G	133	LEU
6	1G	140	ILE
6	1G	159	VAL
6	1G	170	ARG
7	1H	57	ASP
7	1H	76	VAL
7	1H	95	ARG
7	1H	98	LEU
7	1H	116	GLU
7	1H	127	GLU
7	1H	160	LYS
8	1I	6	LEU
8	1I	10	GLU
8	1I	12	LEU
8	1I	20	ASP
8	1I	27	ARG
8	1I	47	LEU
8	1I	58	LEU
8	1I	61	ARG
8	1I	77	LEU
8	1I	85	GLU
8	1I	92	VAL
8	1I	101	LEU
8	1I	102	SER
8	1I	109	ILE
8	1I	123	LEU
8	1I	127	VAL
8	1I	129	THR
8	1I	140	LEU
9	1N	1	MET
9	1N	9	VAL
9	1N	28	THR
9	1N	48	MET
9	1N	61	ARG
9	1N	62	VAL
9	1N	71	ILE
9	1N	84	LYS
10	1O	28	SER
10	1O	42	SER
10	1O	112	MET
11	1P	1	MET
11	1P	65	ARG

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Mol	Chain	Res	Type
11	1P	96	THR
11	1P	98	GLU
11	1P	101	VAL
11	1P	114	ILE
11	1P	147	LEU
11	1P	148	LEU
12	1Q	7	MET
12	1Q	8	LYS
12	1Q	56	ARG
12	1Q	75	THR
12	1Q	109	VAL
12	1Q	133	ARG
13	1R	24	GLN
13	1R	36	THR
13	1R	44	LEU
13	1R	83	ILE
13	1R	100	LEU
13	1R	111	LEU
13	1R	114	VAL
14	1S	3	ARG
14	1S	14	VAL
14	1S	25	ARG
14	1S	69	VAL
15	1T	28	VAL
15	1T	38	ASN
15	1T	82	LEU
15	1T	96	ARG
15	1T	128	GLU
16	1U	17	ILE
16	1U	74	LEU
16	1U	95	LEU
17	1V	53	GLU
17	1V	61	VAL
17	1V	73	SER
17	1V	79	VAL
17	1V	95	LEU
17	1V	100	ARG
18	1W	4	LYS
18	1W	11	ARG
18	1W	15	ARG
18	1W	17	VAL
18	1W	24	ILE

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Mol	Chain	Res	Type
18	1W	67	ASP
19	1X	1	MET
19	1X	37	THR
20	1Y	1	MET
20	1Y	31	LEU
20	1Y	72	VAL
20	1Y	76	CYS
20	1Y	92	ASN
20	1Y	106	LEU
21	1Z	42	VAL
21	1Z	53	ILE
21	1Z	61	LEU
21	1Z	86	VAL
21	1Z	123	ASP
21	1Z	124	ILE
21	1Z	139	VAL
21	1Z	154	ASP
21	1Z	155	LEU
21	1Z	170	THR
21	1Z	171	ILE
23	11	11	ARG
23	11	40	ARG
23	11	59	THR
24	12	1	MET
24	12	19	VAL
24	12	24	LEU
24	12	53	LEU
24	12	55	ARG
25	13	23	LEU
25	13	37	LEU
25	13	54	VAL
26	14	1	MET
26	14	47	GLN
26	14	49	PHE
26	14	52	THR
26	14	53	GLU
26	14	61	ARG
26	14	63	TYR
26	14	67	TYR
27	15	35	GLU
27	15	40	LYS
27	15	55	ARG

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Mol	Chain	Res	Type
27	15	59	GLU
28	16	4	GLU
28	16	6	ARG
28	16	19	ARG
28	16	45	LYS
28	16	47	THR
29	17	24	THR
29	17	43	THR
29	17	46	VAL
30	18	14	VAL
30	18	31	HIS
30	18	34	TRP
31	19	4	ARG
33	1b	12	GLU
33	1b	20	GLU
33	1b	21	ARG
33	1b	23	ARG
33	1b	24	TRP
33	1b	35	GLU
33	1b	37	ASN
33	1b	44	LEU
33	1b	54	THR
33	1b	64	ARG
33	1b	73	THR
33	1b	80	ILE
33	1b	82	ARG
33	1b	101	MET
33	1b	112	VAL
33	1b	127	ILE
33	1b	187	LEU
33	1b	189	ASP
33	1b	196	LEU
33	1b	200	ILE
33	1b	208	ILE
33	1b	212	GLN
33	1b	215	LEU
33	1b	231	GLU
33	1b	236	TYR
34	1c	3	ASN
34	1c	15	THR
34	1c	28	GLN
34	1c	49	SER

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Mol	Chain	Res	Type
34	1c	85	ARG
34	1c	89	GLU
34	1c	98	ASN
34	1c	105	GLU
34	1c	119	ARG
34	1c	124	ILE
34	1c	178	LEU
34	1c	195	VAL
34	1c	201	TYR
34	1c	207	VAL
35	1d	3	ARG
35	1d	19	LEU
35	1d	31	CYS
35	1d	49	ARG
35	1d	59	ARG
35	1d	76	ARG
35	1d	77	ASN
35	1d	86	LYS
35	1d	88	VAL
35	1d	91	SER
35	1d	108	LEU
35	1d	118	ARG
35	1d	127	THR
35	1d	135	LEU
35	1d	144	ASP
35	1d	157	LEU
35	1d	158	ILE
35	1d	170	VAL
35	1d	175	SER
35	1d	177	ASP
35	1d	190	ASP
35	1d	194	LEU
35	1d	200	GLU
36	1e	9	LYS
36	1e	27	ARG
36	1e	41	VAL
36	1e	45	PHE
36	1e	79	GLU
37	1f	19	LEU
37	1f	40	VAL
37	1f	55	ASP
37	1f	57	GLN

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Mol	Chain	Res	Type
37	1f	64	GLN
37	1f	73	ASN
37	1f	75	LEU
37	1f	78	GLU
37	1f	93	SER
38	1g	12	LEU
38	1g	21	VAL
38	1g	24	THR
38	1g	41	ARG
38	1g	50	ILE
38	1g	59	LEU
38	1g	61	VAL
38	1g	85	TYR
38	1g	94	ARG
38	1g	104	LEU
38	1g	110	GLN
38	1g	114	ARG
38	1g	115	ARG
38	1g	155	ARG
39	1h	39	LEU
39	1h	51	VAL
39	1h	52	ASP
39	1h	54	ASP
39	1h	77	GLU
39	1h	86	ILE
39	1h	99	GLU
39	1h	112	LEU
39	1h	133	LEU
40	1i	23	ASN
40	1i	25	LYS
40	1i	27	THR
40	1i	34	ASN
40	1i	50	LEU
40	1i	53	VAL
40	1i	89	ASN
40	1i	96	LEU
40	1i	103	THR
40	1i	105	ASP
40	1i	118	LYS
40	1i	128	ARG
41	1j	23	ILE
41	1j	38	ILE

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Mol	Chain	Res	Type
41	1j	43	ARG
41	1j	81	THR
41	1j	100	THR
42	1k	16	SER
42	1k	25	TYR
42	1k	31	THR
42	1k	48	ILE
42	1k	80	VAL
42	1k	87	THR
42	1k	109	VAL
42	1k	114	VAL
42	1k	117	ASN
43	1l	33	ARG
43	1l	46	LYS
43	1l	83	VAL
44	1m	3	ARG
44	1m	4	ILE
44	1m	11	ARG
44	1m	43	THR
44	1m	49	THR
44	1m	64	TRP
44	1m	70	LEU
44	1m	94	ARG
44	1m	106	ASN
44	1m	109	THR
44	1m	121	LYS
45	1n	3	ARG
45	1n	9	LYS
45	1n	13	THR
45	1n	56	VAL
46	1o	10	LYS
46	1o	11	VAL
46	1o	27	VAL
46	1o	39	LEU
46	1o	76	GLU
46	1o	87	ILE
46	1o	88	ARG
47	1p	20	VAL
47	1p	21	VAL
47	1p	27	LYS
47	1p	43	LYS
47	1p	45	THR

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Mol	Chain	Res	Type
47	1p	48	TRP
47	1p	54	GLU
47	1p	60	LEU
47	1p	62	VAL
47	1p	67	THR
48	1q	11	VAL
48	1q	45	HIS
48	1q	85	VAL
48	1q	86	GLU
48	1q	98	LEU
49	1r	31	LEU
49	1r	35	ARG
49	1r	54	ARG
49	1r	63	GLN
50	1s	4	SER
50	1s	5	LEU
50	1s	28	LYS
50	1s	37	ARG
50	1s	41	VAL
50	1s	66	MET
51	1t	10	LEU
51	1t	24	LEU
51	1t	84	LEU
51	1t	100	ILE
52	1u	15	ARG
52	1u	20	LYS
52	1u	24	ARG
56	1z	5	MET
3	2D	3	VAL
3	2D	20	ASP
3	2D	37	LEU
3	2D	61	LEU
3	2D	88	ARG
3	2D	99	ASP
3	2D	141	VAL
3	2D	142	VAL
3	2D	211	ARG
3	2D	242	ARG
4	2E	38	THR
4	2E	47	VAL
4	2E	72	VAL
4	2E	78	LEU

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Mol	Chain	Res	Type
4	2E	90	THR
4	2E	92	THR
4	2E	113	PHE
4	2E	116	VAL
4	2E	119	ARG
4	2E	154	LYS
4	2E	175	VAL
5	2F	28	ILE
5	2F	33	LEU
5	2F	50	SER
5	2F	74	ARG
5	2F	137	LYS
5	2F	145	GLU
5	2F	162	LEU
5	2F	175	THR
5	2F	179	GLU
5	2F	195	ASP
6	2G	4	ASP
6	2G	18	GLU
6	2G	26	GLN
6	2G	28	VAL
6	2G	31	VAL
6	2G	43	LEU
6	2G	45	GLU
6	2G	49	ASP
6	2G	51	ARG
6	2G	53	LEU
6	2G	60	LEU
6	2G	62	LEU
6	2G	91	ARG
6	2G	109	VAL
6	2G	126	ASP
6	2G	133	LEU
6	2G	140	ILE
6	2G	145	THR
6	2G	170	ARG
7	2H	7	LEU
7	2H	15	VAL
7	2H	24	VAL
7	2H	57	ASP
7	2H	84	SER
7	2H	99	VAL

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Mol	Chain	Res	Type
7	2H	122	THR
7	2H	129	THR
7	2H	130	ARG
8	2I	38	LEU
8	2I	40	THR
8	2I	43	ASN
8	2I	44	LEU
8	2I	50	ARG
8	2I	58	LEU
8	2I	61	ARG
8	2I	68	LEU
8	2I	72	LEU
8	2I	82	ARG
8	2I	86	THR
8	2I	87	LYS
8	2I	102	SER
8	2I	117	GLU
8	2I	127	VAL
8	2I	129	THR
8	2I	133	HIS
8	2I	140	LEU
8	2I	142	VAL
8	2I	145	VAL
9	2N	1	MET
9	2N	28	THR
9	2N	38	HIS
9	2N	60	ILE
9	2N	73	THR
9	2N	83	LYS
9	2N	131	GLN
10	2O	71	ARG
10	2O	104	ARG
11	2P	7	ARG
11	2P	65	ARG
11	2P	77	ARG
11	2P	95	VAL
11	2P	98	GLU
11	2P	100	LEU
11	2P	119	GLU
11	2P	125	VAL
11	2P	133	SER
11	2P	135	LEU

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Mol	Chain	Res	Type
11	2P	147	LEU
11	2P	149	GLU
12	2Q	106	VAL
12	2Q	133	ARG
13	2R	6	SER
13	2R	24	GLN
13	2R	36	THR
13	2R	44	LEU
13	2R	100	LEU
13	2R	111	LEU
13	2R	114	VAL
14	2S	25	ARG
14	2S	26	LEU
14	2S	27	SER
14	2S	43	GLU
14	2S	58	LEU
14	2S	63	THR
14	2S	84	GLN
14	2S	110	LEU
15	2T	9	LEU
15	2T	28	VAL
15	2T	39	ARG
15	2T	64	ARG
15	2T	72	VAL
15	2T	82	LEU
15	2T	89	VAL
15	2T	96	ARG
15	2T	104	ASN
16	2U	5	LYS
16	2U	74	LEU
16	2U	95	LEU
16	2U	111	GLU
16	2U	117	GLN
17	2V	7	THR
17	2V	46	VAL
17	2V	52	VAL
17	2V	61	VAL
17	2V	73	SER
17	2V	82	ARG
17	2V	93	GLU
17	2V	98	GLU
18	2W	4	LYS

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Mol	Chain	Res	Type
18	2W	11	ARG
18	2W	15	ARG
18	2W	17	VAL
18	2W	67	ASP
18	2W	78	GLU
18	2W	92	ARG
19	2X	75	ASP
19	2X	81	VAL
19	2X	92	LEU
20	2Y	1	MET
20	2Y	5	MET
20	2Y	6	HIS
20	2Y	14	LEU
20	2Y	26	LYS
20	2Y	67	LEU
20	2Y	70	SER
20	2Y	72	VAL
20	2Y	90	LEU
20	2Y	91	GLU
20	2Y	97	ARG
20	2Y	98	VAL
20	2Y	99	CYS
21	2Z	33	LEU
21	2Z	35	ARG
21	2Z	41	LEU
21	2Z	42	VAL
21	2Z	53	ILE
21	2Z	63	ASP
21	2Z	67	LEU
21	2Z	70	LEU
21	2Z	71	VAL
21	2Z	91	LEU
21	2Z	96	VAL
21	2Z	100	VAL
21	2Z	121	HIS
21	2Z	122	ARG
21	2Z	144	LEU
21	2Z	151	HIS
21	2Z	153	SER
21	2Z	154	ASP
21	2Z	170	THR
21	2Z	171	ILE

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Mol	Chain	Res	Type
22	20	74	ARG
23	21	11	ARG
23	21	26	ARG
23	21	40	ARG
23	21	59	THR
23	21	89	GLU
24	22	2	LYS
24	22	35	LEU
24	22	45	SER
24	22	70	GLN
25	23	31	LEU
25	23	35	ARG
25	23	54	VAL
25	23	59	VAL
26	24	1	MET
26	24	34	GLU
26	24	50	VAL
26	24	59	PHE
26	24	63	TYR
26	24	67	TYR
27	25	6	VAL
27	25	35	GLU
27	25	55	ARG
28	26	6	ARG
28	26	19	ARG
28	26	23	THR
28	26	28	ARG
28	26	36	LEU
28	26	48	VAL
28	26	52	VAL
29	27	1	MET
29	27	23	ARG
29	27	41	ARG
29	27	46	VAL
30	28	13	ARG
30	28	23	VAL
30	28	31	HIS
33	2b	8	LYS
33	2b	9	GLU
33	2b	11	LEU
33	2b	16	HIS
33	2b	24	TRP

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Mol	Chain	Res	Type
33	2b	35	GLU
33	2b	37	ASN
33	2b	48	MET
33	2b	68	ILE
33	2b	71	VAL
33	2b	76	GLN
33	2b	82	ARG
33	2b	83	MET
33	2b	93	VAL
33	2b	107	THR
33	2b	110	GLN
33	2b	112	VAL
33	2b	115	LEU
33	2b	117	GLU
33	2b	127	ILE
33	2b	138	LEU
33	2b	142	LEU
33	2b	164	VAL
33	2b	169	LYS
33	2b	175	ARG
33	2b	185	ILE
33	2b	187	LEU
33	2b	189	ASP
33	2b	198	ASP
33	2b	209	ARG
33	2b	230	VAL
33	2b	236	TYR
34	2c	3	ASN
34	2c	16	ARG
34	2c	32	LEU
34	2c	34	LEU
34	2c	46	GLU
34	2c	52	LEU
34	2c	91	LEU
34	2c	101	LEU
34	2c	116	VAL
34	2c	132	ARG
34	2c	153	VAL
34	2c	188	LEU
34	2c	190	ARG
34	2c	206	GLU
35	2d	5	ILE

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Mol	Chain	Res	Type
35	2d	18	LYS
35	2d	28	SER
35	2d	31	CYS
35	2d	58	LEU
35	2d	59	ARG
35	2d	76	ARG
35	2d	86	LYS
35	2d	96	LEU
35	2d	127	THR
35	2d	135	LEU
35	2d	150	GLU
35	2d	155	LEU
35	2d	156	GLU
35	2d	158	ILE
35	2d	175	SER
36	2e	13	ILE
36	2e	38	GLN
36	2e	41	VAL
36	2e	51	VAL
36	2e	120	THR
36	2e	150	ARG
36	2e	152	ARG
37	2f	28	ARG
37	2f	64	GLN
37	2f	69	GLU
37	2f	72	VAL
37	2f	81	ILE
37	2f	94	GLN
37	2f	95	GLU
38	2g	6	ARG
38	2g	9	VAL
38	2g	13	GLN
38	2g	15	ASP
38	2g	21	VAL
38	2g	24	THR
38	2g	37	ASN
38	2g	45	ASP
38	2g	78	ARG
38	2g	79	ARG
38	2g	94	ARG
38	2g	98	SER
38	2g	139	GLU

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Mol	Chain	Res	Type
38	2g	154	TYR
39	2h	3	THR
39	2h	18	ARG
39	2h	29	SER
39	2h	37	ARG
39	2h	51	VAL
39	2h	52	ASP
39	2h	54	ASP
39	2h	68	ARG
39	2h	85	ARG
39	2h	99	GLU
39	2h	112	LEU
39	2h	113	SER
39	2h	133	LEU
40	2i	12	GLU
40	2i	23	ASN
40	2i	35	GLU
40	2i	38	GLN
40	2i	40	LEU
40	2i	54	ASP
40	2i	65	VAL
40	2i	66	ARG
40	2i	89	ASN
40	2i	102	LEU
40	2i	113	LYS
40	2i	125	TYR
41	2j	21	GLN
41	2j	23	ILE
41	2j	38	ILE
41	2j	66	ARG
41	2j	67	THR
41	2j	89	ASP
41	2j	97	GLU
42	2k	24	SER
42	2k	41	THR
42	2k	48	ILE
42	2k	62	GLN
42	2k	87	THR
42	2k	105	VAL
42	2k	107	SER
43	2l	28	LYS
43	2l	33	ARG

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Mol	Chain	Res	Type
43	2l	40	VAL
43	2l	47	LYS
43	2l	62	SER
43	2l	65	GLU
44	2m	32	GLU
44	2m	77	ASN
44	2m	90	LEU
44	2m	91	ARG
44	2m	103	THR
44	2m	106	ASN
44	2m	110	ARG
44	2m	114	ARG
45	2n	3	ARG
45	2n	33	VAL
46	2o	13	GLN
46	2o	27	VAL
46	2o	39	LEU
47	2p	20	VAL
47	2p	21	VAL
47	2p	35	LYS
47	2p	42	ARG
47	2p	67	THR
48	2q	5	VAL
48	2q	19	VAL
48	2q	24	GLU
48	2q	60	ILE
48	2q	63	ARG
49	2r	31	LEU
49	2r	56	THR
49	2r	82	THR
50	2s	32	LYS
50	2s	36	ARG
50	2s	37	ARG
50	2s	43	GLU
50	2s	45	VAL
50	2s	47	HIS
50	2s	48	THR
50	2s	49	ILE
50	2s	81	ARG
51	2t	15	ARG
51	2t	17	ARG
51	2t	46	GLU

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Mol	Chain	Res	Type
51	2t	70	SER
51	2t	86	ARG
51	2t	93	GLU
52	2u	7	ARG
56	2z	5	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (117) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	87	ASN
3	1D	116	GLN
4	1E	48	GLN
5	1F	8	GLN
5	1F	69	HIS
6	1G	26	GLN
6	1G	108	ASN
8	1I	133	HIS
10	1O	3	GLN
12	1Q	12	GLN
12	1Q	123	HIS
13	1R	71	GLN
15	1T	58	ASN
16	1U	81	HIS
19	1X	31	HIS
19	1X	82	GLN
21	1Z	55	HIS
21	1Z	73	GLN
21	1Z	132	ASN
21	1Z	151	HIS
24	12	46	GLN
25	13	32	GLN
33	1b	40	HIS
34	1c	6	HIS
34	1c	102	ASN
34	1c	162	GLN
34	1c	170	GLN
35	1d	116	GLN
35	1d	123	HIS
35	1d	125	HIS
36	1e	20	GLN
36	1e	78	HIS
36	1e	141	GLN

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Mol	Chain	Res	Type
37	1f	57	GLN
37	1f	73	ASN
38	1g	13	GLN
38	1g	28	ASN
38	1g	64	GLN
38	1g	86	GLN
39	1h	15	ASN
40	1i	3	GLN
40	1i	31	GLN
40	1i	34	ASN
40	1i	38	GLN
40	1i	58	HIS
40	1i	124	GLN
41	1j	56	HIS
42	1k	93	GLN
43	1l	99	HIS
44	1m	77	ASN
44	1m	92	HIS
49	1r	63	GLN
50	1s	47	HIS
50	1s	57	HIS
50	1s	83	HIS
3	2D	116	GLN
4	2E	48	GLN
5	2F	69	HIS
6	2G	108	ASN
7	2H	74	ASN
8	2I	105	HIS
9	2N	131	GLN
10	2O	5	GLN
12	2Q	12	GLN
14	2S	38	GLN
15	2T	43	GLN
15	2T	84	GLN
15	2T	104	ASN
16	2U	94	ASN
19	2X	31	HIS
19	2X	82	GLN
21	2Z	55	HIS
24	22	46	GLN
24	22	70	GLN
25	23	32	GLN

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Mol	Chain	Res	Type
26	24	46	GLN
31	29	20	HIS
31	29	36	GLN
33	2b	76	GLN
33	2b	95	GLN
33	2b	135	GLN
33	2b	140	HIS
34	2c	37	GLN
34	2c	110	ASN
34	2c	162	GLN
35	2d	45	GLN
35	2d	77	ASN
35	2d	116	GLN
35	2d	119	GLN
35	2d	123	HIS
35	2d	125	HIS
35	2d	161	ASN
36	2e	38	GLN
37	2f	73	ASN
37	2f	94	GLN
37	2f	100	ASN
38	2g	13	GLN
38	2g	28	ASN
38	2g	37	ASN
40	2i	3	GLN
40	2i	31	GLN
40	2i	34	ASN
40	2i	38	GLN
41	2j	13	HIS
41	2j	21	GLN
41	2j	33	GLN
41	2j	62	HIS
42	2k	104	GLN
42	2k	117	ASN
43	2l	49	ASN
43	2l	99	HIS
44	2m	77	ASN
49	2r	63	GLN
50	2s	47	HIS
50	2s	69	HIS
50	2s	83	HIS
51	2t	75	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2863/2915 (98%)	432 (15%)	30 (1%)
1	2A	2790/2915 (95%)	438 (15%)	21 (0%)
2	1B	119/121 (98%)	9 (7%)	0
2	2B	118/121 (97%)	21 (17%)	0
32	1a	1494/1521 (98%)	231 (15%)	0
32	2a	1498/1521 (98%)	273 (18%)	0
53	1v	12/24 (50%)	1 (8%)	0
53	2v	12/24 (50%)	3 (25%)	0
54	1w	70/76 (92%)	23 (32%)	0
54	2w	67/76 (88%)	20 (29%)	0
55	1x	75/77 (97%)	5 (6%)	0
55	2x	75/77 (97%)	9 (12%)	0
57	1y	71/76 (93%)	29 (40%)	0
57	2y	69/76 (90%)	19 (27%)	0
All	All	9333/9620 (97%)	1513 (16%)	51 (0%)

All (1513) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	34	C
1	1A	45	C
1	1A	63	U
1	1A	71	A
1	1A	74	A
1	1A	75	G
1	1A	84	A
1	1A	118	A
1	1A	119	A
1	1A	120	U
1	1A	140	G
1	1A	151	C
1	1A	154(A)	C
1	1A	181	A
1	1A	182	A
1	1A	188	G
1	1A	196	A
1	1A	197	A
1	1A	205	G
1	1A	215	G
1	1A	216	A
1	1A	222	A

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Mol	Chain	Res	Type
1	1A	229	A
1	1A	233	A
1	1A	248	G
1	1A	265	A
1	1A	269	U
1	1A	271(B)	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	271(X)	G
1	1A	272(A)	U
1	1A	272(B)	G
1	1A	272(H)	C
1	1A	275	G
1	1A	279	C
1	1A	283	A
1	1A	311	A
1	1A	327	G
1	1A	329	G
1	1A	330	A
1	1A	352	G
1	1A	353	G
1	1A	357	A
1	1A	363	G
1	1A	363(A)	A
1	1A	363(B)	G
1	1A	386	G
1	1A	389	G
1	1A	396	G
1	1A	405	U
1	1A	411	G
1	1A	428	A
1	1A	444	C
1	1A	448	U
1	1A	451	C
1	1A	456	C
1	1A	479	A
1	1A	481	G
1	1A	504	U

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Mol	Chain	Res	Type
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	586	A
1	1A	592	G
1	1A	603	A
1	1A	604	G
1	1A	607	U
1	1A	615	G
1	1A	616	G
1	1A	627	A
1	1A	637	A
1	1A	645	C
1	1A	646	A
1	1A	652(D)	C
1	1A	652(E)	G
1	1A	652(F)	G
1	1A	652(T)	C
1	1A	669	G
1	1A	686	G
1	1A	717	G
1	1A	730	C
1	1A	765	G
1	1A	775	G
1	1A	776	G
1	1A	782	A
1	1A	784	A
1	1A	785	G
1	1A	789	A
1	1A	792	G
1	1A	805	G
1	1A	812	C
1	1A	819	A

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Mol	Chain	Res	Type
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	892	G
1	1A	893	C
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
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	1040	C
1	1A	1044	G
1	1A	1046	A

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Mol	Chain	Res	Type
1	1A	1047	G
1	1A	1048	A
1	1A	1054	A
1	1A	1055	G
1	1A	1058	G
1	1A	1059	G
1	1A	1063	G
1	1A	1064	C
1	1A	1065	U
1	1A	1068	G
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	1081	U
1	1A	1083	U
1	1A	1088	A
1	1A	1090	U
1	1A	1091	G
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	1111	A
1	1A	1112	G
1	1A	1117	G
1	1A	1135	C
1	1A	1136	G
1	1A	1142	U
1	1A	1149	G
1	1A	1170	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

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Mol	Chain	Res	Type
1	1A	1178	C
1	1A	1220	A
1	1A	1229	G
1	1A	1236	G
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	1319	G
1	1A	1342	A
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	1395	A
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	1445	A
1	1A	1450	G
1	1A	1455	G
1	1A	1459	G
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

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Mol	Chain	Res	Type
1	1A	1509	C
1	1A	1509(A)	A
1	1A	1525	G
1	1A	1539	G
1	1A	1554	A
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	1608	A
1	1A	1609	A
1	1A	1610	A
1	1A	1647	G
1	1A	1648	C
1	1A	1674	G
1	1A	1696	G
1	1A	1700	A
1	1A	1703	G
1	1A	1722	A
1	1A	1746	G
1	1A	1756	G
1	1A	1762	A
1	1A	1763	G
1	1A	1764	G
1	1A	1769	G
1	1A	1773	A
1	1A	1780	A
1	1A	1782	C
1	1A	1791	A
1	1A	1800	C
1	1A	1801	G
1	1A	1812	A
1	1A	1816	G
1	1A	1828	G
1	1A	1829	A
1	1A	1847	A
1	1A	1877	A
1	1A	1878	G
1	1A	1889	A

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Mol	Chain	Res	Type
1	1A	1900	A
1	1A	1906	G
1	1A	1929	G
1	1A	1930	G
1	1A	1937	A
1	1A	1938	A
1	1A	1955	U
1	1A	1963	U
1	1A	1967	C
1	1A	1970	A
1	1A	1971	A
1	1A	1972	A
1	1A	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	2039	C
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	2108	C
1	1A	2110	G
1	1A	2112	G
1	1A	2113	U
1	1A	2114	A
1	1A	2116	G
1	1A	2117	A
1	1A	2118	U
1	1A	2120	G
1	1A	2121	G
1	1A	2123	G
1	1A	2126	A
1	1A	2127	G
1	1A	2129	C

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Mol	Chain	Res	Type
1	1A	2130	U
1	1A	2131	G
1	1A	2132	U
1	1A	2133	G
1	1A	2134	A
1	1A	2135	A
1	1A	2136	C
1	1A	2137	C
1	1A	2140	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	2167	U
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	2193	G
1	1A	2198	A
1	1A	2206	G
1	1A	2207	G
1	1A	2219	G
1	1A	2225	A
1	1A	2238	G
1	1A	2268	A
1	1A	2283	C
1	1A	2287	A

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Mol	Chain	Res	Type
1	1A	2289	G
1	1A	2305	A
1	1A	2308	G
1	1A	2320	A
1	1A	2322	A
1	1A	2325	G
1	1A	2334	G
1	1A	2347	C
1	1A	2350	C
1	1A	2361	A
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	2424	C
1	1A	2425	A
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
1	1A	2505	G
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	2611	U

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Mol	Chain	Res	Type
1	1A	2612	C
1	1A	2629	A
1	1A	2630	G
1	1A	2654	A
1	1A	2686	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	2758	A
1	1A	2760	C
1	1A	2765	A
1	1A	2778	A
1	1A	2790	A
1	1A	2791	C
1	1A	2793	G
1	1A	2802	G
1	1A	2803	C
1	1A	2820	A
1	1A	2821	A
1	1A	2835	A
1	1A	2872	G
1	1A	2880	C
1	1A	2892	A
1	1A	2894	G
2	1B	13	A
2	1B	25	A
2	1B	45	A
2	1B	56	G
2	1B	57	A
2	1B	67	G
2	1B	73	A
2	1B	85	G
2	1B	110	G
32	1a	7	G

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Mol	Chain	Res	Type
32	1a	9	G
32	1a	32	A
32	1a	39	G
32	1a	47	C
32	1a	48	C
32	1a	50	A
32	1a	51	A
32	1a	54	C
32	1a	61	G
32	1a	73	G
32	1a	77	G
32	1a	79	G
32	1a	91	C
32	1a	98	G
32	1a	101	A
32	1a	105	G
32	1a	116	A
32	1a	121	C
32	1a	131	C
32	1a	144	G
32	1a	163	C
32	1a	164	U
32	1a	174	C
32	1a	176	C
32	1a	182	U
32	1a	189	G
32	1a	189(C)	C
32	1a	189(J)	G
32	1a	195	A
32	1a	197	A
32	1a	202	U
32	1a	203	U
32	1a	204	U
32	1a	216	G
32	1a	247	G
32	1a	251	G
32	1a	266	G
32	1a	267	C
32	1a	280	C
32	1a	289	G
32	1a	321	A
32	1a	328	C

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Mol	Chain	Res	Type
32	1a	330	C
32	1a	332	G
32	1a	344	A
32	1a	347	G
32	1a	351	G
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	384	G
32	1a	390	C
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	430	A
32	1a	439	A
32	1a	441	A
32	1a	442	C
32	1a	452	A
32	1a	461	A
32	1a	470	C
32	1a	471	G
32	1a	474	G
32	1a	483	C
32	1a	485	G
32	1a	493	G
32	1a	496	A
32	1a	498	U
32	1a	509	A
32	1a	510	A
32	1a	511	C
32	1a	518	C
32	1a	521	G
32	1a	531	U

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Mol	Chain	Res	Type
32	1a	532	A
32	1a	547	A
32	1a	559	A
32	1a	561	U
32	1a	564	C
32	1a	568	G
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	577	G
32	1a	596	C
32	1a	607	A
32	1a	630	G
32	1a	653	A
32	1a	657	G
32	1a	665	A
32	1a	666	G
32	1a	687	A
32	1a	688	G
32	1a	703	G
32	1a	723	U
32	1a	731	G
32	1a	734	G
32	1a	749	C
32	1a	752	G
32	1a	755	G
32	1a	773	G
32	1a	777	A
32	1a	792	A
32	1a	793	U
32	1a	794	A
32	1a	816	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	874	G
32	1a	914	A
32	1a	916	G
32	1a	926	G

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Mol	Chain	Res	Type
32	1a	927	G
32	1a	934	C
32	1a	935	A
32	1a	942	G
32	1a	960	U
32	1a	961	U
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	972	C
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	1003	G
32	1a	1005	A
32	1a	1006	C
32	1a	1008	C
32	1a	1011	G
32	1a	1020	U
32	1a	1022	G
32	1a	1023	G
32	1a	1024	G
32	1a	1025	U
32	1a	1026	G
32	1a	1027	C
32	1a	1028	C
32	1a	1029	C
32	1a	1030	C
32	1a	1030(A)	G
32	1a	1030(C)	G
32	1a	1031	G
32	1a	1033	G
32	1a	1039	C
32	1a	1044	A
32	1a	1068	G
32	1a	1081	G
32	1a	1094	G

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Mol	Chain	Res	Type
32	1a	1095	U
32	1a	1101	A
32	1a	1108	G
32	1a	1111	A
32	1a	1124	G
32	1a	1125	U
32	1a	1127	G
32	1a	1132	C
32	1a	1134	G
32	1a	1136	U
32	1a	1137	C
32	1a	1138	G
32	1a	1139	G
32	1a	1146	A
32	1a	1152	A
32	1a	1159	U
32	1a	1183	A
32	1a	1184	G
32	1a	1196	U
32	1a	1197	G
32	1a	1202	G
32	1a	1214	C
32	1a	1227	A
32	1a	1236	A
32	1a	1238	A
32	1a	1256	A
32	1a	1257	U
32	1a	1258	G
32	1a	1270	C
32	1a	1275	A
32	1a	1278	U
32	1a	1279	A
32	1a	1280	A
32	1a	1282	C
32	1a	1286	A
32	1a	1287	A
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1319	A
32	1a	1323	G
32	1a	1346	A

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Mol	Chain	Res	Type
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1364	U
32	1a	1370	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	1492	A
32	1a	1494	G
32	1a	1503	A
32	1a	1504	G
32	1a	1506	U
32	1a	1517	G
32	1a	1529	G
32	1a	1530	G
32	1a	1531	A
53	1v	13	A
54	1w	2	C
54	1w	6	G
54	1w	7	A
54	1w	8	4SU
54	1w	14	A
54	1w	19	G
54	1w	20	U
54	1w	21	A
54	1w	23	A
54	1w	24	G
54	1w	25	C
54	1w	34	G
54	1w	45	U
54	1w	46	G7M
54	1w	47	U
54	1w	48	C
54	1w	50	U
54	1w	61	C
54	1w	67	C
54	1w	68	C
54	1w	70	G

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Mol	Chain	Res	Type
54	1w	73	A
54	1w	74	C
55	1x	9	G
55	1x	21	A
55	1x	47	U
55	1x	61	C
55	1x	64	G
57	1y	5	G
57	1y	6	G
57	1y	7	A
57	1y	9	A
57	1y	13	C
57	1y	14	A
57	1y	19	G
57	1y	20	U
57	1y	21	A
57	1y	35	A
57	1y	39	PSU
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	50	U
57	1y	52	G
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	62	C
57	1y	65	G
57	1y	70	G
57	1y	72	C
1	2A	12	U
1	2A	15	G
1	2A	34	C
1	2A	35	G
1	2A	45	C
1	2A	49	A

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Mol	Chain	Res	Type
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	79	G
1	2A	84	A
1	2A	90	U
1	2A	94	C
1	2A	95	G
1	2A	100	G
1	2A	102	G
1	2A	118	A
1	2A	119	A
1	2A	120	U
1	2A	123	G
1	2A	154	G
1	2A	154(A)	C
1	2A	157	U
1	2A	181	A
1	2A	196	A
1	2A	199	A
1	2A	205	G
1	2A	214	G
1	2A	215	G
1	2A	216	A
1	2A	222	A
1	2A	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(K)	U
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	271(O)	C
1	2A	272(B)	G
1	2A	274	G
1	2A	277	C
1	2A	278	A
1	2A	294	A
1	2A	311	A

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Mol	Chain	Res	Type
1	2A	324	A
1	2A	327	G
1	2A	329	G
1	2A	330	A
1	2A	352	G
1	2A	363	G
1	2A	363(B)	G
1	2A	363(C)	G
1	2A	386	G
1	2A	389	G
1	2A	396	G
1	2A	403	U
1	2A	411	G
1	2A	421	U
1	2A	435	C
1	2A	443	A
1	2A	444	C
1	2A	454	A
1	2A	455	C
1	2A	457	A
1	2A	481	G
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	551	G
1	2A	563	G
1	2A	573	G
1	2A	575	A
1	2A	588	U
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	614(B)	G
1	2A	615	G
1	2A	616	G
1	2A	627	A
1	2A	634	C

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Mol	Chain	Res	Type
1	2A	637	A
1	2A	643	A
1	2A	645	C
1	2A	652(B)	A
1	2A	652(C)	G
1	2A	669	G
1	2A	686	G
1	2A	717	G
1	2A	726	G
1	2A	730	C
1	2A	752	A
1	2A	753	C
1	2A	775	G
1	2A	776	G
1	2A	782	A
1	2A	784	A
1	2A	785	G
1	2A	790	C
1	2A	792	G
1	2A	805	G
1	2A	812	C
1	2A	819	A
1	2A	827	U
1	2A	828	U
1	2A	854	G
1	2A	857	C
1	2A	859	G
1	2A	874	G
1	2A	879	G
1	2A	880	G
1	2A	882	G
1	2A	884	C
1	2A	886	C
1	2A	887	A
1	2A	888	C
1	2A	889	C
1	2A	893	C
1	2A	894	C
1	2A	896	A
1	2A	900	A
1	2A	901	A
1	2A	904	C

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Mol	Chain	Res	Type
1	2A	910	A
1	2A	917	A
1	2A	932	G
1	2A	941	A
1	2A	945	A
1	2A	946	G
1	2A	953	A
1	2A	959	A
1	2A	961	C
1	2A	974	G
1	2A	975	C
1	2A	983	A
1	2A	996	A
1	2A	999	U
1	2A	1012	U
1	2A	1013	C
1	2A	1017	G
1	2A	1022	G
1	2A	1025	G
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	1143	A
1	2A	1167	U
1	2A	1169	G
1	2A	1171	G
1	2A	1181	C
1	2A	1195	G
1	2A	1205	U
1	2A	1210	A
1	2A	1211	U
1	2A	1212	G
1	2A	1220	A
1	2A	1224	C
1	2A	1229	G

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Mol	Chain	Res	Type
1	2A	1248	G
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A
1	2A	1300	U
1	2A	1301	A
1	2A	1314	C
1	2A	1359	A
1	2A	1360	A
1	2A	1365	A
1	2A	1370	C
1	2A	1380	G
1	2A	1384	A
1	2A	1385	G
1	2A	1395	A
1	2A	1416	G
1	2A	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	1463	C
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	1496	A
1	2A	1497	U
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1523	U

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Mol	Chain	Res	Type
1	2A	1531	C
1	2A	1532	C
1	2A	1543	C
1	2A	1547	C
1	2A	1558	A
1	2A	1559	G
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1580	A
1	2A	1584	C
1	2A	1608	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	1721	G
1	2A	1722	A
1	2A	1739	U
1	2A	1740	G
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	1812	A
1	2A	1816	G
1	2A	1829	A
1	2A	1835	G
1	2A	1847	A
1	2A	1848	A
1	2A	1858	G
1	2A	1861	G
1	2A	1866	C

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Mol	Chain	Res	Type
1	2A	1877	A
1	2A	1878	G
1	2A	1900	A
1	2A	1906	G
1	2A	1929	G
1	2A	1930	G
1	2A	1936	A
1	2A	1938	A
1	2A	1955	U
1	2A	1963	U
1	2A	1965	C
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1984	G
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	2113	U
1	2A	2116	G
1	2A	2117	A
1	2A	2119	A
1	2A	2120	G
1	2A	2122	U
1	2A	2124	G
1	2A	2126	A
1	2A	2127	G

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Mol	Chain	Res	Type
1	2A	2128	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	2144	U
1	2A	2145	C
1	2A	2150	U
1	2A	2151	G
1	2A	2153	G
1	2A	2155	G
1	2A	2156	G
1	2A	2157	G
1	2A	2158	A
1	2A	2159	G
1	2A	2161	C
1	2A	2163	C
1	2A	2166	G
1	2A	2167	U
1	2A	2168	G
1	2A	2169	A
1	2A	2172	U
1	2A	2174	C
1	2A	2176	A
1	2A	2178	C
1	2A	2181	G
1	2A	2183	C
1	2A	2184	G
1	2A	2185	C
1	2A	2189	U
1	2A	2190	G
1	2A	2193	G
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2225	A
1	2A	2239	G

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Mol	Chain	Res	Type
1	2A	2268	A
1	2A	2275	C
1	2A	2278	A
1	2A	2280	G
1	2A	2283	C
1	2A	2287	A
1	2A	2289	G
1	2A	2298	A
1	2A	2305	A
1	2A	2308	G
1	2A	2319	G
1	2A	2320	A
1	2A	2325	G
1	2A	2327	A
1	2A	2334	G
1	2A	2336	A
1	2A	2347	C
1	2A	2350	C
1	2A	2354	G
1	2A	2372	G
1	2A	2376	A
1	2A	2383	G
1	2A	2385	C
1	2A	2403	C
1	2A	2406	U
1	2A	2414	G
1	2A	2424	C
1	2A	2425	A
1	2A	2429	G
1	2A	2430	A
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2445	G
1	2A	2448	A
1	2A	2465	C
1	2A	2469	A
1	2A	2476	A
1	2A	2491	U
1	2A	2494	G
1	2A	2502	G
1	2A	2505	G

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Mol	Chain	Res	Type
1	2A	2506	U
1	2A	2507	C
1	2A	2518	A
1	2A	2520	C
1	2A	2525	G
1	2A	2529	G
1	2A	2530	A
1	2A	2532	G
1	2A	2534	A
1	2A	2554	U
1	2A	2566	A
1	2A	2567	G
1	2A	2573	C
1	2A	2578	G
1	2A	2582	G
1	2A	2585	U
1	2A	2602	A
1	2A	2609	U
1	2A	2611	U
1	2A	2612	C
1	2A	2630	G
1	2A	2634	G
1	2A	2641	G
1	2A	2654	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	2751	G
1	2A	2758	A
1	2A	2765	A
1	2A	2766	G
1	2A	2778	A
1	2A	2789	C
1	2A	2793	G
1	2A	2802	G
1	2A	2803	C

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Mol	Chain	Res	Type
1	2A	2808	U
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	2892	A
1	2A	2894	G
1	2A	2897	U
2	2B	2	C
2	2B	3	C
2	2B	8	U
2	2B	12	C
2	2B	13	A
2	2B	17	C
2	2B	34	U
2	2B	41	U
2	2B	45	A
2	2B	53	A
2	2B	73	A
2	2B	74	U
2	2B	75	G
2	2B	84	C
2	2B	88	C
2	2B	89	G
2	2B	106	G
2	2B	109	C
2	2B	110	G
2	2B	113	G
2	2B	120	A
32	2a	9	G
32	2a	22	G
32	2a	32	A
32	2a	39	G
32	2a	41	G
32	2a	47	C
32	2a	48	C
32	2a	50	A
32	2a	51	A

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Mol	Chain	Res	Type
32	2a	56	U
32	2a	66	G
32	2a	70	G
32	2a	78	G
32	2a	79	G
32	2a	80	G
32	2a	88	A
32	2a	89	C
32	2a	101	A
32	2a	116	A
32	2a	121	C
32	2a	131	C
32	2a	144	G
32	2a	156	G
32	2a	159	G
32	2a	162	A
32	2a	163	C
32	2a	182	U
32	2a	189(C)	C
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	247	G
32	2a	251	G
32	2a	258	G
32	2a	266	G
32	2a	267	C
32	2a	281	G
32	2a	289	G
32	2a	301	G
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	350	G
32	2a	351	G
32	2a	352	C
32	2a	353	A

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Mol	Chain	Res	Type
32	2a	354	G
32	2a	356	A
32	2a	367	U
32	2a	372	C
32	2a	384	G
32	2a	388	G
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	412	A
32	2a	413	G
32	2a	421	U
32	2a	423	G
32	2a	424	G
32	2a	429	U
32	2a	439	A
32	2a	442	C
32	2a	449	C
32	2a	452	A
32	2a	461	A
32	2a	470	C
32	2a	471	G
32	2a	484	G
32	2a	485	G
32	2a	496	A
32	2a	498	U
32	2a	505	G
32	2a	509	A
32	2a	510	A
32	2a	511	C
32	2a	518	C
32	2a	527	G7M
32	2a	531	U
32	2a	532	A
32	2a	533	A
32	2a	547	A
32	2a	559	A
32	2a	564	C
32	2a	568	G
32	2a	572	A
32	2a	573	A
32	2a	574	A

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Mol	Chain	Res	Type
32	2a	576	G
32	2a	577	G
32	2a	596	C
32	2a	630	G
32	2a	653	A
32	2a	665	A
32	2a	666	G
32	2a	671	G
32	2a	687	A
32	2a	688	G
32	2a	695	A
32	2a	703	G
32	2a	723	U
32	2a	724	G
32	2a	731	G
32	2a	733	A
32	2a	749	C
32	2a	755	G
32	2a	777	A
32	2a	787	A
32	2a	793	U
32	2a	794	A
32	2a	817	C
32	2a	821	G
32	2a	827	U
32	2a	828	A
32	2a	834	C
32	2a	840	C
32	2a	841	U
32	2a	859	A
32	2a	874	G
32	2a	902	G
32	2a	914	A
32	2a	926	G
32	2a	927	G
32	2a	934	C
32	2a	935	A
32	2a	939	G
32	2a	942	G
32	2a	960	U
32	2a	961	U
32	2a	968	A

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Mol	Chain	Res	Type
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	983	A
32	2a	992	U
32	2a	993	G
32	2a	995	C
32	2a	997	U
32	2a	998	G
32	2a	999	C
32	2a	1002	G
32	2a	1003	G
32	2a	1005	A
32	2a	1006	C
32	2a	1007	C
32	2a	1008	C
32	2a	1009	G
32	2a	1011	G
32	2a	1016	A
32	2a	1019	C
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	1029	C
32	2a	1030	C
32	2a	1030(A)	G
32	2a	1031	G
32	2a	1032	G
32	2a	1033	G
32	2a	1035	A
32	2a	1036	G
32	2a	1037	C

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Mol	Chain	Res	Type
32	2a	1039	C
32	2a	1040	U
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	1097	C
32	2a	1101	A
32	2a	1104	G
32	2a	1105	A
32	2a	1117	G
32	2a	1122	U
32	2a	1124	G
32	2a	1125	U
32	2a	1129	C
32	2a	1130	A
32	2a	1133	G
32	2a	1136	U
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G
32	2a	1140	C
32	2a	1141	C
32	2a	1146	A
32	2a	1152	A
32	2a	1157	A
32	2a	1159	U
32	2a	1160	G
32	2a	1182	G
32	2a	1184	G
32	2a	1191	A
32	2a	1193	G
32	2a	1196	U
32	2a	1197	G

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Mol	Chain	Res	Type
32	2a	1202	G
32	2a	1211	U
32	2a	1213	A
32	2a	1220	G
32	2a	1227	A
32	2a	1238	A
32	2a	1240	U
32	2a	1241	G
32	2a	1246	C
32	2a	1248	A
32	2a	1255	G
32	2a	1256	A
32	2a	1257	U
32	2a	1260	C
32	2a	1261	A
32	2a	1270	C
32	2a	1272	G
32	2a	1273	G
32	2a	1277	C
32	2a	1278	U
32	2a	1279	A
32	2a	1280	A
32	2a	1285	A
32	2a	1287	A
32	2a	1299	A
32	2a	1302	U
32	2a	1303	C
32	2a	1305	G
32	2a	1320	C
32	2a	1323	G
32	2a	1338	G
32	2a	1346	A
32	2a	1347	G
32	2a	1358	U
32	2a	1363	C
32	2a	1364	U
32	2a	1368	G
32	2a	1370	G
32	2a	1380	U
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G

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Mol	Chain	Res	Type
32	2a	1447	A
32	2a	1452	C
32	2a	1456	G
32	2a	1492	A
32	2a	1494	G
32	2a	1504	G
32	2a	1506	U
32	2a	1517	G
32	2a	1529	G
32	2a	1530	G
32	2a	1531	A
32	2a	1532	U
53	2v	14	A
53	2v	15	A
53	2v	19	U
54	2w	3	C
54	2w	4	C
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	27	G
54	2w	46	G7M
54	2w	47	U
54	2w	48	C
54	2w	58	A
54	2w	62	C
54	2w	65	G
54	2w	68	C
54	2w	69	G
54	2w	70	G
54	2w	74	C
55	2x	9	G
55	2x	13	C
55	2x	18	G
55	2x	20	U
55	2x	21	A
55	2x	47	U
55	2x	51	C

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Mol	Chain	Res	Type
55	2x	56	C
55	2x	69	C
57	2y	8	4SU
57	2y	15	G
57	2y	19	G
57	2y	27	G
57	2y	43	C
57	2y	45	U
57	2y	49	C
57	2y	52	G
57	2y	53	G
57	2y	54	5MU
57	2y	56	C
57	2y	58	A
57	2y	59	U
57	2y	61	C
57	2y	65	G
57	2y	69	G
57	2y	70	G
57	2y	73	A
57	2y	75	C

All (51) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	196	A
1	1A	266	G
1	1A	271(J)	C
1	1A	278	A
1	1A	548	A
1	1A	746	A
1	1A	764	A
1	1A	774	A
1	1A	974	G
1	1A	1047	G
1	1A	1067	A
1	1A	1142(A)	A
1	1A	1174	A
1	1A	1176	G
1	1A	1275	A
1	1A	1379	A
1	1A	1442	G

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Mol	Chain	Res	Type
1	1A	1508	A
1	1A	1608	A
1	1A	1992	G
1	1A	1997	G
1	1A	2134	A
1	1A	2183	C
1	1A	2406	U
1	1A	2422	A
1	1A	2430	A
1	1A	2439	A
1	1A	2629	A
1	1A	2689	U
1	1A	2756	U
1	2A	196	A
1	2A	228	A
1	2A	266	G
1	2A	271(M)	G
1	2A	277	C
1	2A	528	A
1	2A	752	A
1	2A	827	U
1	2A	856	C
1	2A	900	A
1	2A	1210	A
1	2A	1379	A
1	2A	1420	U
1	2A	1442	G
1	2A	1530	C
1	2A	1653	G
1	2A	1992	G
1	2A	2119	A
1	2A	2126	A
1	2A	2439	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	MA6	1a	1519	32	19,26,27	0.83	0	18,38,41	1.51	2 (11%)
57	G7M	1y	46	57	20,26,27	1.36	2 (10%)	17,39,42	0.56	0
55	5MC	1x	32	55	18,22,23	1.01	2 (11%)	26,32,35	1.22	3 (11%)
1	PSU	1A	1917	1	18,21,22	1.41	3 (16%)	22,30,33	1.83	4 (18%)
57	PSU	2y	39	57	18,21,22	1.27	2 (11%)	22,30,33	2.08	4 (18%)
1	5MU	2A	1915	1	19,22,23	1.44	5 (26%)	28,32,35	2.11	6 (21%)
57	MIA	1y	37	57	18,24,32	1.14	2 (11%)	18,35,47	1.23	2 (11%)
55	PSU	1x	55	55	18,21,22	1.40	2 (11%)	22,30,33	1.89	3 (13%)
32	M2G	1a	966	32	20,27,28	1.43	3 (15%)	22,40,43	1.10	3 (13%)
54	PSU	2w	39	54	18,21,22	1.34	2 (11%)	22,30,33	1.69	3 (13%)
57	PSU	1y	32	57	18,21,22	1.35	2 (11%)	22,30,33	1.82	4 (18%)
55	5MU	1x	54	55	19,22,23	1.41	4 (21%)	28,32,35	1.97	6 (21%)
55	4SU	1x	8	55	18,21,22	2.15	6 (33%)	26,30,33	1.71	7 (26%)
1	PSU	1A	2605	1,58	18,21,22	1.37	2 (11%)	22,30,33	2.08	4 (18%)
57	5MU	1y	54	57	19,22,23	1.43	5 (26%)	28,32,35	1.70	6 (21%)
57	MIA	2y	37	57	18,24,32	1.12	2 (11%)	18,35,47	1.32	2 (11%)
32	2MG	1a	1207	32	18,26,27	1.03	1 (5%)	16,38,41	1.02	1 (6%)
32	4OC	2a	1402	32	20,23,24	0.77	0	26,32,35	1.00	1 (3%)
55	5MC	2x	32	55	18,22,23	0.95	2 (11%)	26,32,35	1.21	4 (15%)
1	OMG	1A	2251	1,58,55	18,26,27	0.94	1 (5%)	19,38,41	1.07	2 (10%)
54	F3N	1w	76	1,54	30,36,37	1.53	5 (16%)	29,51,54	1.23	1 (3%)
32	MA6	2a	1519	32	19,26,27	0.82	0	18,38,41	1.62	2 (11%)
32	5MC	2a	1400	32	18,22,23	0.96	2 (11%)	26,32,35	1.20	3 (11%)
32	5MC	1a	1407	32	18,22,23	0.93	2 (11%)	26,32,35	1.06	1 (3%)
32	5MC	2a	1404	32	18,22,23	0.99	2 (11%)	26,32,35	1.12	2 (7%)
32	G7M	1a	527	32	20,26,27	1.21	2 (10%)	17,39,42	0.61	0
54	MIA	1w	37	54	24,31,32	2.03	3 (12%)	26,44,47	3.01	9 (34%)
55	5MU	2x	54	55	19,22,23	1.38	5 (26%)	28,32,35	2.15	6 (21%)
54	PSU	2w	32	54	18,21,22	1.31	2 (11%)	22,30,33	1.81	3 (13%)
32	UR3	1a	1498	32	19,22,23	0.96	0	26,32,35	1.46	2 (7%)
55	8AN	1x	76	55,58	19,24,25	1.32	4 (21%)	13,35,38	1.92	2 (15%)
54	G7M	1w	46	54	20,26,27	1.25	2 (10%)	17,39,42	0.81	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MC	1A	1942	1	18,22,23	1.00	2 (11%)	26,32,35	1.19	3 (11%)
1	OMG	2A	2251	1,58,55	18,26,27	0.95	1 (5%)	19,38,41	1.21	3 (15%)
57	4SU	2y	8	57	18,21,22	1.63	4 (22%)	26,30,33	2.09	5 (19%)
57	PSU	2y	55	57	18,21,22	1.34	2 (11%)	22,30,33	1.85	4 (18%)
43	0TD	2l	92	43	7,9,10	4.74	1 (14%)	6,11,13	4.55	3 (50%)
32	MA6	1a	1518	32	19,26,27	0.83	0	18,38,41	1.53	2 (11%)
1	5MC	2A	1942	1	18,22,23	0.97	2 (11%)	26,32,35	1.14	2 (7%)
54	PSU	2w	55	54	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
32	MA6	2a	1518	32	19,26,27	0.84	0	18,38,41	1.51	2 (11%)
1	PSU	1A	1911	1	18,21,22	1.39	2 (11%)	22,30,33	1.99	3 (13%)
1	5MC	2A	1962	1,58	18,22,23	0.94	2 (11%)	26,32,35	1.13	2 (7%)
32	5MC	1a	1404	32	18,22,23	1.01	2 (11%)	26,32,35	1.27	4 (15%)
32	PSU	2a	516	32	18,21,22	1.30	2 (11%)	22,30,33	1.88	3 (13%)
43	0TD	1l	92	43	7,9,10	4.93	1 (14%)	6,11,13	7.84	3 (50%)
56	FME	1z	1	56	8,9,10	0.94	0	7,9,11	1.24	1 (14%)
54	5MU	1w	54	54	19,22,23	1.32	5 (26%)	28,32,35	1.96	6 (21%)
54	5MU	2w	54	54	19,22,23	1.32	4 (21%)	28,32,35	1.84	6 (21%)
1	OMU	2A	2552	1,58	19,22,23	1.17	2 (10%)	26,31,34	1.78	6 (23%)
32	5MC	2a	967	32	18,22,23	0.94	2 (11%)	26,32,35	1.08	2 (7%)
1	5MU	1A	1915	1	19,22,23	1.37	5 (26%)	28,32,35	2.14	7 (25%)
32	5MC	2a	1407	32	18,22,23	0.95	2 (11%)	26,32,35	1.13	2 (7%)
32	4OC	1a	1402	32	20,23,24	0.73	0	26,32,35	1.07	2 (7%)
1	2MA	1A	2503	1,58	17,25,26	1.04	1 (5%)	17,37,40	0.99	2 (11%)
1	PSU	2A	1917	1	18,21,22	1.37	2 (11%)	22,30,33	1.89	3 (13%)
54	PSU	1w	32	58,54	18,21,22	1.27	2 (11%)	22,30,33	1.89	4 (18%)
54	4SU	2w	8	54	18,21,22	1.67	3 (16%)	26,30,33	2.34	5 (19%)
57	4SU	1y	8	57	18,21,22	1.66	4 (22%)	26,30,33	1.90	5 (19%)
1	5MU	1A	1939	1,58	19,22,23	1.37	4 (21%)	28,32,35	2.39	6 (21%)
1	PSU	2A	2605	1	18,21,22	1.32	4 (22%)	22,30,33	1.85	3 (13%)
55	4SU	2x	8	55,58	18,21,22	2.03	4 (22%)	26,30,33	1.47	6 (23%)
1	5MU	2A	1939	1,58	19,22,23	1.37	5 (26%)	28,32,35	2.32	8 (28%)
54	MIA	2w	37	54	20,27,32	1.74	2 (10%)	22,39,47	1.95	7 (31%)
57	G7M	2y	46	57	20,26,27	1.42	2 (10%)	17,39,42	0.77	1 (5%)
32	PSU	1a	516	32	18,21,22	1.33	2 (11%)	22,30,33	1.80	3 (13%)
57	5MU	2y	54	57	19,22,23	1.52	4 (21%)	28,32,35	2.18	6 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	2A	1911	1	18,21,22	1.37	2 (11%)	22,30,33	1.93	4 (18%)
54	PSU	1w	55	54	18,21,22	1.36	2 (11%)	22,30,33	1.80	3 (13%)
1	2MA	2A	2503	1,58	17,25,26	1.05	1 (5%)	17,37,40	0.94	2 (11%)
56	FME	2z	1	56	8,9,10	0.97	0	7,9,11	1.05	0
54	4SU	1w	8	58,54	18,21,22	1.77	5 (27%)	26,30,33	1.85	5 (19%)
1	5MC	1A	1962	1,58	18,22,23	0.92	2 (11%)	26,32,35	1.16	3 (11%)
32	UR3	2a	1498	32	19,22,23	1.08	1 (5%)	26,32,35	1.46	3 (11%)
1	OMC	2A	1920	1	19,22,23	0.83	0	26,31,34	0.91	0
57	PSU	1y	39	57	18,21,22	1.33	2 (11%)	22,30,33	1.89	3 (13%)
1	OMU	1A	2552	1,58	19,22,23	1.21	2 (10%)	26,31,34	1.82	4 (15%)
57	PSU	1y	55	57	18,21,22	1.33	2 (11%)	22,30,33	1.87	3 (13%)
54	PSU	1w	39	54	18,21,22	1.32	2 (11%)	22,30,33	1.84	3 (13%)
55	8AN	2x	76	55,58	19,24,25	1.20	3 (15%)	13,35,38	1.94	3 (23%)
32	5MC	1a	967	32	18,22,23	0.92	2 (11%)	26,32,35	1.14	3 (11%)
1	OMC	1A	1920	1	19,22,23	0.84	0	26,31,34	1.01	2 (7%)
32	M2G	2a	966	32	20,27,28	1.46	3 (15%)	22,40,43	1.04	3 (13%)
54	F3N	2w	76	1,54	30,36,37	1.42	5 (16%)	29,51,54	1.27	2 (6%)
57	PSU	2y	32	57	18,21,22	1.36	2 (11%)	22,30,33	1.73	3 (13%)
32	2MG	2a	1207	32	18,26,27	0.94	1 (5%)	16,38,41	1.03	1 (6%)
55	PSU	2x	55	55	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
32	5MC	1a	1400	32	18,22,23	0.96	2 (11%)	26,32,35	1.15	2 (7%)
54	G7M	2w	46	54	20,26,27	1.17	1 (5%)	17,39,42	0.80	0
32	G7M	2a	527	32,58	20,26,27	1.23	2 (10%)	17,39,42	0.57	0

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	MA6	1a	1519	32	-	3/7/29/30	0/3/3/3
57	G7M	1y	46	57	-	2/3/25/26	0/3/3/3
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
57	PSU	2y	39	57	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
57	MIA	1y	37	57	-	1/3/25/34	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
57	PSU	1y	32	57	-	1/7/25/26	0/2/2/2
55	5MU	1x	54	55	-	0/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
1	PSU	1A	2605	1,58	-	0/7/25/26	0/2/2/2
57	5MU	1y	54	57	-	0/7/25/26	0/2/2/2
57	MIA	2y	37	57	-	1/3/25/34	0/3/3/3
32	2MG	1a	1207	32	-	0/5/27/28	0/3/3/3
32	4OC	2a	1402	32	-	0/9/29/30	0/2/2/2
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
1	OMG	1A	2251	1,58,55	-	1/5/27/28	0/3/3/3
54	F3N	1w	76	1,54	-	0/15/37/38	0/4/4/4
32	MA6	2a	1519	32	-	3/7/29/30	0/3/3/3
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
32	G7M	1a	527	32	-	3/3/25/26	0/3/3/3
54	MIA	1w	37	54	-	4/11/33/34	0/3/3/3
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
54	PSU	2w	32	54	-	2/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
55	8AN	1x	76	55,58	-	3/3/25/26	0/3/3/3
54	G7M	1w	46	54	-	1/3/25/26	0/3/3/3
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	1,58,55	-	0/5/27/28	0/3/3/3
57	4SU	2y	8	57	-	1/7/25/26	0/2/2/2
57	PSU	2y	55	57	-	1/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	2/7/12/14	-
32	MA6	1a	1518	32	-	0/7/29/30	0/3/3/3
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	0/7/29/30	0/3/3/3
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	1,58	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	1/7/12/14	-
56	FME	1z	1	56	-	4/7/9/11	-
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
1	OMU	2A	2552	1,58	-	0/9/27/28	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
1	5MU	1A	1915	1	-	0/7/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	0/9/29/30	0/2/2/2
1	2MA	1A	2503	1,58	-	2/3/25/26	0/3/3/3
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
54	PSU	1w	32	58,54	-	0/7/25/26	0/2/2/2
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2
57	4SU	1y	8	57	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	1,58	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
55	4SU	2x	8	55,58	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	1,58	-	0/7/25/26	0/2/2/2
54	MIA	2w	37	54	-	2/7/29/34	0/3/3/3
57	G7M	2y	46	57	-	2/3/25/26	0/3/3/3
32	PSU	1a	516	32	-	0/7/25/26	0/2/2/2
57	5MU	2y	54	57	-	2/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	1,58	-	1/3/25/26	0/3/3/3
56	FME	2z	1	56	-	3/7/9/11	-
54	4SU	1w	8	58,54	-	0/7/25/26	0/2/2/2
1	5MC	1A	1962	1,58	-	0/7/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
57	PSU	1y	39	57	-	0/7/25/26	0/2/2/2
1	OMU	1A	2552	1,58	-	0/9/27/28	0/2/2/2
57	PSU	1y	55	57	-	2/7/25/26	0/2/2/2
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
55	8AN	2x	76	55,58	-	3/3/25/26	0/3/3/3
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
1	OMC	1A	1920	1	-	1/9/27/28	0/2/2/2
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
54	F3N	2w	76	1,54	-	3/15/37/38	0/4/4/4
57	PSU	2y	32	57	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	0/5/27/28	0/3/3/3
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	G7M	2w	46	54	-	1/3/25/26	0/3/3/3
32	G7M	2a	527	32,58	-	3/3/25/26	0/3/3/3

All (203) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-12.65	1.69	1.82
43	2l	92	0TD	CB-SB	-12.23	1.69	1.82
54	1w	37	MIA	C13-C14	6.97	1.52	1.32
54	2w	37	MIA	C2-S10	-6.47	1.70	1.75
54	1w	37	MIA	C2-S10	-5.48	1.71	1.75
55	1x	8	4SU	C4-N3	-5.19	1.32	1.37
54	1w	76	F3N	CB-CG	-4.87	1.39	1.51
55	2x	8	4SU	C4-N3	-4.81	1.32	1.37
32	2a	966	M2G	C2-N3	4.79	1.36	1.30
54	2w	76	F3N	CB-CG	-4.61	1.40	1.51
32	1a	966	M2G	C2-N3	4.56	1.36	1.30
54	2w	8	4SU	C4-S4	-4.54	1.59	1.68
54	1w	8	4SU	C4-S4	-4.33	1.60	1.68
57	2y	46	G7M	C5-C4	4.33	1.47	1.39
57	2y	8	4SU	C4-S4	-4.22	1.60	1.68
57	1y	8	4SU	C4-S4	-4.21	1.60	1.68
55	2x	8	4SU	C4-S4	-4.17	1.60	1.68
57	1y	46	G7M	C5-C4	4.10	1.47	1.39
55	1x	8	4SU	C4-S4	-4.09	1.60	1.68
54	1w	76	F3N	O4'-C1'	3.91	1.46	1.41
57	1y	39	PSU	C6-C5	3.88	1.39	1.35
57	2y	32	PSU	C6-C5	3.84	1.39	1.35
54	1w	55	PSU	C6-C5	3.78	1.39	1.35
55	1x	8	4SU	C2-N3	-3.76	1.31	1.38
54	1w	46	G7M	C5-C4	3.76	1.46	1.39
32	1a	527	G7M	C5-C4	3.76	1.46	1.39
57	1y	32	PSU	C6-C5	3.74	1.39	1.35
32	2a	527	G7M	C5-C4	3.68	1.46	1.39
54	2w	55	PSU	C6-C5	3.65	1.39	1.35
54	2w	46	G7M	C5-C4	3.63	1.46	1.39
57	1y	55	PSU	C6-C5	3.54	1.39	1.35
1	1A	1917	PSU	C6-C5	3.51	1.39	1.35
55	2x	55	PSU	C6-C5	3.50	1.39	1.35
55	1x	55	PSU	C6-C5	3.46	1.39	1.35
55	1x	8	4SU	C5-C4	-3.39	1.38	1.42
54	1w	8	4SU	C4-N3	-3.39	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2a	516	PSU	C6-C5	3.38	1.39	1.35
54	2w	32	PSU	C6-C5	3.38	1.39	1.35
1	2A	1917	PSU	C6-C5	3.38	1.39	1.35
54	2w	39	PSU	C6-C5	3.34	1.39	1.35
54	1w	32	PSU	C6-C5	3.32	1.39	1.35
55	2x	8	4SU	C2-N3	-3.30	1.32	1.38
57	2y	39	PSU	C6-C5	3.27	1.39	1.35
1	1A	1911	PSU	C6-C5	3.18	1.39	1.35
1	2A	1911	PSU	C6-C5	3.17	1.39	1.35
57	2y	55	PSU	C6-C5	3.15	1.39	1.35
57	2y	54	5MU	C2-N1	3.15	1.43	1.38
32	1a	516	PSU	C6-C5	3.13	1.39	1.35
57	2y	54	5MU	C6-C5	3.12	1.39	1.34
55	2x	8	4SU	C5-C4	-3.10	1.38	1.42
32	1a	966	M2G	C2-N2	3.07	1.41	1.35
54	1w	39	PSU	C6-C5	3.03	1.38	1.35
32	1a	1207	2MG	C6-N1	-2.98	1.33	1.37
57	1y	54	5MU	C6-C5	2.95	1.39	1.34
1	1A	2605	PSU	C6-C5	2.92	1.38	1.35
1	2A	1942	5MC	C6-C5	2.89	1.39	1.34
54	2w	8	4SU	C4-N3	-2.88	1.34	1.37
1	2A	1915	5MU	C6-C5	2.88	1.39	1.34
54	2w	76	F3N	O4'-C1'	2.88	1.45	1.41
55	1x	32	5MC	C6-C5	2.87	1.39	1.34
1	1A	1911	PSU	C4-N3	-2.84	1.33	1.38
1	1A	1917	PSU	C4-N3	-2.84	1.33	1.38
32	2a	1404	5MC	C6-C5	2.84	1.39	1.34
55	1x	76	8AN	C5-C4	-2.84	1.33	1.40
55	2x	76	8AN	C5-C4	-2.84	1.33	1.40
1	1A	1942	5MC	C6-C5	2.83	1.39	1.34
32	1a	1404	5MC	C6-C5	2.82	1.39	1.34
1	2A	2605	PSU	C6-C5	2.80	1.38	1.35
1	1A	2552	OMU	C4-N3	-2.79	1.33	1.38
32	1a	1400	5MC	C6-C5	2.79	1.39	1.34
57	1y	8	4SU	C4-N3	-2.79	1.34	1.37
1	1A	2605	PSU	C4-N3	-2.78	1.33	1.38
32	2a	1400	5MC	C6-C5	2.78	1.39	1.34
55	1x	54	5MU	C6-C5	2.77	1.39	1.34
54	2w	76	F3N	C5-C4	-2.76	1.33	1.40
54	1w	76	F3N	C5-C4	-2.76	1.33	1.40
57	1y	37	MIA	C5-C4	2.75	1.48	1.40
55	2x	54	5MU	C6-C5	2.75	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	2y	8	4SU	C4-N3	-2.74	1.34	1.37
54	1w	39	PSU	C4-N3	-2.74	1.33	1.38
57	1y	37	MIA	C2-N3	2.72	1.36	1.32
57	1y	54	5MU	C4-N3	-2.70	1.33	1.38
32	1a	1407	5MC	C6-C5	2.70	1.39	1.34
55	2x	32	5MC	C6-C5	2.69	1.39	1.34
54	1w	8	4SU	C5-C4	-2.68	1.39	1.42
57	2y	46	G7M	C6-N1	-2.67	1.33	1.37
57	2y	37	MIA	C5-C4	2.66	1.48	1.40
57	2y	54	5MU	C4-C5	2.65	1.49	1.44
1	2A	1917	PSU	C4-N3	-2.64	1.33	1.38
1	2A	1962	5MC	C6-C5	2.62	1.38	1.34
57	2y	37	MIA	C2-N3	2.61	1.36	1.32
1	2A	1911	PSU	C4-N3	-2.61	1.34	1.38
1	1A	1915	5MU	C4-N3	-2.60	1.34	1.38
54	1w	37	MIA	C5-C4	2.60	1.47	1.40
32	2a	967	5MC	C6-C5	2.60	1.38	1.34
1	1A	1939	5MU	C6-C5	2.59	1.38	1.34
55	2x	55	PSU	C4-N3	-2.59	1.34	1.38
55	1x	54	5MU	C4-N3	-2.59	1.34	1.38
1	2A	2251	OMG	C6-N1	-2.58	1.34	1.37
32	2a	966	M2G	C6-N1	-2.56	1.34	1.37
1	2A	1939	5MU	C4-C5	2.56	1.49	1.44
1	1A	1939	5MU	C4-C5	2.56	1.49	1.44
1	1A	2251	OMG	C6-N1	-2.56	1.34	1.37
1	2A	1915	5MU	C4-C5	2.56	1.49	1.44
1	2A	1915	5MU	C2-N1	2.55	1.42	1.38
54	2w	39	PSU	C4-N3	-2.54	1.34	1.38
1	2A	1939	5MU	C6-C5	2.54	1.38	1.34
1	2A	1939	5MU	C6-N1	-2.54	1.33	1.38
55	1x	55	PSU	C4-N3	-2.54	1.34	1.38
32	2a	966	M2G	C2-N2	2.54	1.39	1.35
54	2w	54	5MU	C6-C5	2.53	1.38	1.34
54	1w	54	5MU	C6-C5	2.53	1.38	1.34
54	1w	76	F3N	C6-C5	-2.52	1.33	1.43
32	1a	516	PSU	C4-N3	-2.51	1.34	1.38
54	2w	76	F3N	C6-C5	-2.51	1.34	1.43
55	2x	76	8AN	C6-C5	-2.51	1.34	1.43
55	2x	54	5MU	C4-N3	-2.51	1.34	1.38
1	1A	2503	2MA	C2-N3	2.51	1.36	1.31
55	1x	76	8AN	C6-C5	-2.50	1.34	1.43
54	2w	37	MIA	C5-C4	2.50	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1915	5MU	C6-C5	2.50	1.38	1.34
55	1x	54	5MU	C2-N1	2.50	1.42	1.38
54	1w	46	G7M	C6-N1	-2.49	1.34	1.37
1	2A	1915	5MU	C4-N3	-2.47	1.34	1.38
57	1y	32	PSU	C4-N3	-2.46	1.34	1.38
32	1a	1404	5MC	C6-N1	-2.44	1.33	1.38
32	2a	1407	5MC	C6-C5	2.43	1.38	1.34
32	2a	1407	5MC	C6-N1	-2.42	1.33	1.38
1	2A	1962	5MC	C6-N1	-2.41	1.33	1.38
1	2A	1939	5MU	C4-N3	-2.40	1.34	1.38
1	2A	2552	OMU	C4-N3	-2.40	1.34	1.38
1	1A	1962	5MC	C6-C5	2.38	1.38	1.34
1	1A	1942	5MC	C6-N1	-2.38	1.34	1.38
54	2w	8	4SU	C5-C4	-2.38	1.39	1.42
32	2a	1207	2MG	C6-N1	-2.36	1.34	1.37
1	2A	2503	2MA	C2-N3	2.35	1.36	1.31
57	1y	54	5MU	C2-N1	2.35	1.42	1.38
57	2y	8	4SU	C5-C4	-2.35	1.39	1.42
54	2w	54	5MU	C4-N3	-2.34	1.34	1.38
1	1A	1915	5MU	C2-N1	2.34	1.42	1.38
57	1y	55	PSU	C4-N3	-2.34	1.34	1.38
57	2y	54	5MU	C4-N3	-2.34	1.34	1.38
1	1A	1939	5MU	C6-N1	-2.34	1.34	1.38
32	1a	967	5MC	C6-N1	-2.33	1.34	1.38
57	2y	39	PSU	C4-N3	-2.33	1.34	1.38
54	2w	55	PSU	C4-N3	-2.33	1.34	1.38
1	2A	2605	PSU	C4-N3	-2.33	1.34	1.38
55	2x	32	5MC	C6-N1	-2.33	1.34	1.38
57	1y	8	4SU	C2-N1	2.33	1.42	1.38
55	1x	32	5MC	C6-N1	-2.32	1.34	1.38
32	2a	1400	5MC	C6-N1	-2.32	1.34	1.38
54	1w	54	5MU	C4-N3	-2.32	1.34	1.38
54	1w	55	PSU	C4-N3	-2.31	1.34	1.38
57	2y	55	PSU	C4-N3	-2.31	1.34	1.38
57	2y	32	PSU	C4-N3	-2.31	1.34	1.38
1	1A	2552	OMU	C5-C4	2.30	1.48	1.43
32	1a	1400	5MC	C6-N1	-2.30	1.34	1.38
32	1a	967	5MC	C6-C5	2.30	1.38	1.34
54	1w	54	5MU	C2-N1	2.30	1.42	1.38
54	1w	32	PSU	C4-N3	-2.28	1.34	1.38
55	1x	54	5MU	C4-C5	2.28	1.48	1.44
1	1A	1962	5MC	C6-N1	-2.27	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2w	32	PSU	C4-N3	-2.27	1.34	1.38
55	1x	8	4SU	O2-C2	2.26	1.27	1.23
32	2a	1498	UR3	C2-N1	2.26	1.41	1.38
55	2x	54	5MU	C4-C5	2.26	1.48	1.44
57	1y	39	PSU	C4-N3	-2.25	1.34	1.38
54	1w	8	4SU	C2-N1	2.23	1.42	1.38
57	1y	8	4SU	C5-C4	-2.23	1.39	1.42
32	2a	967	5MC	C6-N1	-2.22	1.34	1.38
1	1A	1915	5MU	C6-N1	-2.22	1.34	1.38
32	2a	516	PSU	C4-N3	-2.21	1.34	1.38
55	2x	54	5MU	C2-N1	2.21	1.42	1.38
57	1y	46	G7M	C6-N1	-2.20	1.34	1.37
54	2w	54	5MU	C4-C5	2.20	1.48	1.44
57	1y	54	5MU	C4-C5	2.19	1.48	1.44
1	1A	1939	5MU	C2-N3	-2.19	1.34	1.38
32	2a	527	G7M	C6-N1	-2.18	1.34	1.37
55	1x	76	8AN	O4'-C1'	2.18	1.44	1.41
54	1w	8	4SU	C2-N3	-2.17	1.34	1.38
54	2w	76	F3N	C5-N7	-2.17	1.31	1.39
54	2w	54	5MU	C2-N1	2.16	1.41	1.38
57	2y	8	4SU	C2-N1	2.14	1.41	1.38
32	1a	1407	5MC	C6-N1	-2.13	1.34	1.38
1	1A	1915	5MU	C4-C5	2.12	1.48	1.44
1	2A	2605	PSU	C2-N1	-2.11	1.33	1.36
1	2A	2552	OMU	C5-C4	2.11	1.48	1.43
54	1w	76	F3N	C5-N7	-2.10	1.32	1.39
54	1w	54	5MU	C6-N1	-2.09	1.34	1.38
55	2x	76	8AN	C5-N7	-2.08	1.32	1.39
32	2a	1404	5MC	C6-N1	-2.08	1.34	1.38
1	1A	1917	PSU	C2-N3	-2.06	1.34	1.37
1	2A	1939	5MU	C2-N3	-2.06	1.34	1.38
55	2x	54	5MU	C6-N1	-2.05	1.34	1.38
57	1y	54	5MU	C6-N1	-2.03	1.34	1.38
55	1x	76	8AN	C5-N7	-2.03	1.32	1.39
32	1a	966	M2G	C6-N1	-2.03	1.34	1.37
32	1a	527	G7M	C6-N1	-2.02	1.34	1.37
1	2A	1915	5MU	C6-N1	-2.02	1.34	1.38
54	1w	54	5MU	C4-C5	2.01	1.48	1.44
55	1x	8	4SU	C6-C5	2.00	1.39	1.35
1	2A	2605	PSU	C2-N3	-2.00	1.34	1.37
1	2A	1942	5MC	C6-N1	-2.00	1.34	1.38

All (287) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1l	92	0TD	CSB-SB-CB	-18.72	68.58	102.44
43	2l	92	0TD	CSB-SB-CB	-10.37	83.67	102.44
54	1w	37	MIA	C12-C13-C14	-9.58	108.50	127.14
54	2w	8	4SU	C4-N3-C2	-7.39	120.16	127.34
1	1A	2605	PSU	N1-C2-N3	6.73	122.75	115.13
54	2w	8	4SU	C5-C4-N3	6.43	120.65	114.69
1	1A	1911	PSU	N1-C2-N3	6.31	122.28	115.13
54	1w	37	MIA	C12-N6-C6	-6.30	113.22	122.55
57	2y	39	PSU	N1-C2-N3	6.28	122.25	115.13
57	2y	8	4SU	C4-N3-C2	-6.19	121.32	127.34
1	2A	1911	PSU	N1-C2-N3	6.14	122.08	115.13
1	2A	1917	PSU	N1-C2-N3	5.98	121.91	115.13
32	1a	1498	UR3	C4-N3-C2	-5.94	118.97	124.56
55	1x	55	PSU	N1-C2-N3	5.94	121.86	115.13
54	1w	39	PSU	N1-C2-N3	5.90	121.82	115.13
1	1A	1939	5MU	C4-N3-C2	-5.88	119.74	127.35
54	2w	55	PSU	N1-C2-N3	5.87	121.78	115.13
57	1y	39	PSU	N1-C2-N3	5.83	121.73	115.13
54	1w	32	PSU	N1-C2-N3	5.78	121.68	115.13
32	2a	1498	UR3	C4-N3-C2	-5.76	119.14	124.56
1	2A	1939	5MU	C4-N3-C2	-5.76	119.89	127.35
55	2x	55	PSU	N1-C2-N3	5.74	121.63	115.13
57	1y	55	PSU	N1-C2-N3	5.72	121.61	115.13
1	1A	2552	OMU	N3-C2-N1	5.72	122.48	114.89
32	2a	516	PSU	N1-C2-N3	5.69	121.58	115.13
55	1x	76	8AN	N3-C2-N1	-5.66	119.83	128.68
55	2x	76	8AN	N3-C2-N1	-5.64	119.86	128.68
1	1A	1917	PSU	N1-C2-N3	5.63	121.51	115.13
54	1w	76	F3N	N3-C2-N1	-5.60	119.93	128.68
54	2w	76	F3N	N3-C2-N1	-5.59	119.94	128.68
57	2y	55	PSU	N1-C2-N3	5.57	121.44	115.13
54	2w	32	PSU	N1-C2-N3	5.56	121.43	115.13
54	1w	55	PSU	N1-C2-N3	5.53	121.39	115.13
57	2y	54	5MU	N3-C2-N1	5.51	122.20	114.89
57	1y	8	4SU	C4-N3-C2	-5.44	122.06	127.34
57	2y	54	5MU	C4-N3-C2	-5.44	120.31	127.35
32	1a	516	PSU	N1-C2-N3	5.43	121.28	115.13
54	1w	8	4SU	C5-C4-N3	5.41	119.71	114.69
57	1y	32	PSU	N1-C2-N3	5.40	121.24	115.13
1	1A	1915	5MU	C4-N3-C2	-5.38	120.39	127.35
55	2x	54	5MU	C4-N3-C2	-5.37	120.40	127.35
57	1y	8	4SU	C5-C4-N3	5.37	119.67	114.69
54	2w	39	PSU	N1-C2-N3	5.35	121.19	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	2y	32	PSU	N1-C2-N3	5.30	121.14	115.13
57	2y	8	4SU	C5-C4-N3	5.30	119.61	114.69
1	2A	1915	5MU	C4-N3-C2	-5.29	120.51	127.35
1	1A	1939	5MU	C5-C4-N3	5.27	119.81	115.31
1	1A	1939	5MU	O4-C4-C5	-5.26	118.81	124.90
1	2A	2605	PSU	N1-C2-N3	5.25	121.07	115.13
55	2x	54	5MU	N3-C2-N1	5.24	121.84	114.89
32	1a	1518	MA6	N3-C2-N1	-5.17	120.59	128.68
32	2a	1518	MA6	N3-C2-N1	-5.10	120.71	128.68
32	2a	1519	MA6	N3-C2-N1	-5.09	120.72	128.68
1	2A	1915	5MU	N3-C2-N1	5.04	121.58	114.89
1	1A	1939	5MU	C5-C6-N1	-4.97	118.23	123.34
1	2A	1939	5MU	C5-C4-N3	4.97	119.55	115.31
1	1A	1915	5MU	C5-C4-N3	4.93	119.52	115.31
54	1w	8	4SU	C4-N3-C2	-4.89	122.59	127.34
32	1a	1519	MA6	N3-C2-N1	-4.89	121.04	128.68
54	1w	37	MIA	C15-C14-C13	-4.88	108.53	122.65
1	1A	1915	5MU	N3-C2-N1	4.88	121.36	114.89
55	1x	54	5MU	C4-N3-C2	-4.86	121.06	127.35
1	2A	1939	5MU	N3-C2-N1	4.83	121.31	114.89
55	1x	54	5MU	N3-C2-N1	4.79	121.25	114.89
54	1w	54	5MU	C4-N3-C2	-4.72	121.24	127.35
54	1w	37	MIA	C2-N3-C4	4.69	121.78	115.32
1	2A	2552	OMU	N3-C2-N1	4.65	121.06	114.89
1	2A	1915	5MU	C5-C4-N3	4.62	119.25	115.31
57	2y	39	PSU	C4-N3-C2	-4.58	119.74	126.34
54	1w	54	5MU	N3-C2-N1	4.55	120.92	114.89
1	1A	1939	5MU	N3-C2-N1	4.54	120.92	114.89
1	1A	2605	PSU	C4-N3-C2	-4.51	119.84	126.34
54	1w	54	5MU	O4-C4-C5	-4.50	119.69	124.90
1	2A	1939	5MU	C5-C6-N1	-4.49	118.72	123.34
57	2y	54	5MU	C5-C4-N3	4.47	119.13	115.31
55	2x	54	5MU	C5-C4-N3	4.46	119.11	115.31
55	1x	8	4SU	C6-C5-C4	-4.38	116.16	119.95
1	2A	2552	OMU	C4-N3-C2	-4.32	120.88	126.58
55	2x	54	5MU	O4-C4-C5	-4.27	119.95	124.90
1	1A	1911	PSU	O2-C2-N1	-4.25	118.11	122.79
1	1A	1915	5MU	O4-C4-C5	-4.24	119.98	124.90
54	2w	54	5MU	C4-N3-C2	-4.24	121.86	127.35
54	2w	37	MIA	C2-N3-C4	4.22	121.15	115.32
54	2w	54	5MU	C5-C4-N3	4.20	118.90	115.31
57	1y	54	5MU	N3-C2-N1	4.19	120.45	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	1x	54	5MU	C5-C4-N3	4.19	118.89	115.31
57	2y	54	5MU	O4-C4-C5	-4.17	120.07	124.90
54	1w	54	5MU	C5-C4-N3	4.16	118.86	115.31
1	2A	1939	5MU	O4-C4-C5	-4.14	120.11	124.90
32	2a	1400	5MC	C5-C6-N1	-4.12	119.10	123.34
54	2w	8	4SU	N3-C2-N1	4.11	120.34	114.89
1	2A	1915	5MU	O4-C4-C5	-4.10	120.14	124.90
54	2w	54	5MU	O4-C4-C5	-4.10	120.15	124.90
1	2A	1911	PSU	C4-N3-C2	-4.08	120.45	126.34
57	2y	8	4SU	N3-C2-N1	4.07	120.30	114.89
1	2A	1939	5MU	O2-C2-N1	-4.04	117.42	122.79
55	2x	55	PSU	C4-N3-C2	-4.03	120.53	126.34
1	1A	2552	OMU	O2-C2-N1	-4.02	117.44	122.79
32	2a	516	PSU	C4-N3-C2	-4.02	120.55	126.34
54	2w	8	4SU	C5-C4-S4	-4.00	119.31	124.47
57	1y	39	PSU	C4-N3-C2	-3.98	120.60	126.34
55	2x	32	5MC	C5-C6-N1	-3.97	119.25	123.34
54	1w	32	PSU	C4-N3-C2	-3.95	120.65	126.34
1	1A	1911	PSU	C4-N3-C2	-3.93	120.68	126.34
55	1x	8	4SU	O2-C2-N1	3.92	128.00	122.79
1	1A	2552	OMU	C4-N3-C2	-3.91	121.42	126.58
1	2A	1917	PSU	C4-N3-C2	-3.90	120.73	126.34
54	1w	39	PSU	C4-N3-C2	-3.89	120.73	126.34
57	2y	55	PSU	C4-N3-C2	-3.88	120.74	126.34
54	2w	54	5MU	N3-C2-N1	3.87	120.02	114.89
1	2A	1962	5MC	C5-C6-N1	-3.85	119.37	123.34
1	2A	2605	PSU	C4-N3-C2	-3.84	120.81	126.34
54	2w	37	MIA	C11-S10-C2	-3.81	99.42	102.27
32	1a	516	PSU	C4-N3-C2	-3.80	120.86	126.34
55	1x	54	5MU	O4-C4-C5	-3.78	120.52	124.90
54	2w	32	PSU	C4-N3-C2	-3.78	120.90	126.34
32	1a	1400	5MC	C5-C6-N1	-3.78	119.45	123.34
55	1x	32	5MC	C5-C6-N1	-3.77	119.46	123.34
55	1x	55	PSU	C4-N3-C2	-3.76	120.92	126.34
54	2w	55	PSU	O2-C2-N1	-3.73	118.68	122.79
57	1y	55	PSU	O2-C2-N1	-3.71	118.71	122.79
57	1y	54	5MU	C4-N3-C2	-3.69	122.57	127.35
54	2w	55	PSU	C4-N3-C2	-3.68	121.03	126.34
55	2x	54	5MU	C5-C6-N1	-3.66	119.58	123.34
54	2w	37	MIA	C12-N6-C6	-3.64	119.74	122.87
1	1A	1917	PSU	C4-N3-C2	-3.62	121.12	126.34
1	2A	1942	5MC	C5-C6-N1	-3.59	119.64	123.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	1y	32	PSU	C4-N3-C2	-3.59	121.16	126.34
57	2y	39	PSU	O2-C2-N1	-3.59	118.84	122.79
32	2a	1407	5MC	C5-C6-N1	-3.57	119.67	123.34
1	2A	2605	PSU	O2-C2-N1	-3.56	118.87	122.79
55	2x	8	4SU	C5-C4-N3	3.55	117.98	114.69
32	2a	516	PSU	O2-C2-N1	-3.54	118.89	122.79
54	1w	37	MIA	C16-C14-C13	-3.54	112.41	122.65
57	2y	8	4SU	C5-C4-S4	-3.53	119.92	124.47
57	2y	55	PSU	O2-C2-N1	-3.49	118.94	122.79
57	2y	32	PSU	C4-N3-C2	-3.49	121.31	126.34
55	1x	54	5MU	C5-C6-N1	-3.49	119.75	123.34
55	1x	55	PSU	O2-C2-N1	-3.47	118.97	122.79
57	1y	55	PSU	C4-N3-C2	-3.46	121.35	126.34
1	1A	1942	5MC	C5-C6-N1	-3.45	119.78	123.34
54	1w	32	PSU	O2-C2-N1	-3.45	118.99	122.79
54	2w	37	MIA	C5-C6-N1	-3.44	117.95	120.81
57	1y	37	MIA	N3-C2-N1	-3.43	123.31	128.68
1	2A	1915	5MU	C5-C6-N1	-3.43	119.81	123.34
54	2w	32	PSU	O2-C2-N1	-3.41	119.04	122.79
32	1a	1407	5MC	C5-C6-N1	-3.39	119.85	123.34
54	1w	55	PSU	C4-N3-C2	-3.39	121.46	126.34
57	1y	54	5MU	C5-C4-N3	3.38	118.20	115.31
54	2w	39	PSU	C4-N3-C2	-3.38	121.47	126.34
1	1A	2605	PSU	O2-C2-N1	-3.37	119.08	122.79
1	2A	1917	PSU	O2-C2-N1	-3.34	119.11	122.79
54	1w	37	MIA	C5-C6-N1	-3.33	118.05	120.81
1	1A	1962	5MC	C5-C6-N1	-3.33	119.91	123.34
1	2A	1911	PSU	O2-C2-N1	-3.32	119.14	122.79
1	1A	1915	5MU	C5-C6-N1	-3.32	119.93	123.34
54	1w	55	PSU	O2-C2-N1	-3.30	119.16	122.79
1	1A	1939	5MU	O2-C2-N1	-3.30	118.41	122.79
57	1y	32	PSU	O2-C2-N1	-3.27	119.19	122.79
32	2a	1404	5MC	C5-C6-N1	-3.27	119.97	123.34
32	2a	967	5MC	C5-C6-N1	-3.26	119.99	123.34
1	2A	2552	OMU	O2-C2-N1	-3.23	118.50	122.79
57	1y	54	5MU	O4-C4-C5	-3.22	121.17	124.90
54	1w	37	MIA	C2-N1-C6	3.21	122.93	117.19
54	1w	8	4SU	C5-C4-S4	-3.20	120.34	124.47
32	1a	1404	5MC	C5-C6-N1	-3.20	120.05	123.34
57	1y	8	4SU	N3-C2-N1	3.20	119.13	114.89
55	1x	8	4SU	C5-C4-N3	3.19	117.65	114.69
43	1l	92	0TD	OD2-CG-CB	3.18	120.03	113.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	2x	8	4SU	C6-C5-C4	-3.18	117.20	119.95
57	2y	54	5MU	C5-C6-N1	-3.18	120.06	123.34
57	1y	39	PSU	O2-C2-N1	-3.18	119.29	122.79
57	2y	37	MIA	N3-C2-N1	-3.18	123.71	128.68
32	1a	1404	5MC	C5-C4-N3	-3.14	118.28	121.67
57	1y	8	4SU	C5-C4-S4	-3.14	120.42	124.47
32	2a	1519	MA6	C4-C5-N7	-3.13	106.14	109.40
55	2x	8	4SU	C1'-N1-C2	3.12	123.22	117.57
32	1a	1519	MA6	C4-C5-N7	-3.11	106.16	109.40
32	1a	516	PSU	O2-C2-N1	-3.10	119.38	122.79
43	2l	92	0TD	OD2-CG-CB	3.10	119.84	113.15
57	2y	37	MIA	C4-C5-N7	-3.06	106.21	109.40
55	2x	76	8AN	O4'-C1'-C2'	-3.04	102.49	106.93
1	1A	1917	PSU	O2-C2-N1	-3.03	119.46	122.79
32	2a	1518	MA6	C4-C5-N7	-3.02	106.25	109.40
54	1w	37	MIA	C4-C5-N7	-3.02	106.25	109.40
55	1x	32	5MC	C5-C4-N3	-3.01	118.43	121.67
1	2A	2552	OMU	O4-C4-C5	-2.96	119.95	125.16
32	1a	967	5MC	C5-C6-N1	-2.96	120.29	123.34
55	1x	76	8AN	O4'-C1'-C2'	-2.96	102.61	106.93
54	1w	8	4SU	N3-C2-N1	2.94	118.79	114.89
55	1x	8	4SU	S4-C4-N3	-2.89	117.36	120.21
1	2A	2552	OMU	C5-C4-N3	2.86	119.12	114.84
54	1w	37	MIA	N3-C2-N1	-2.85	121.73	126.98
57	2y	32	PSU	O2-C2-N1	-2.85	119.65	122.79
54	2w	76	F3N	C3'-N3'-C	-2.84	118.94	123.21
54	2w	54	5MU	C5-C6-N1	-2.83	120.42	123.34
54	1w	54	5MU	C5-C6-N1	-2.79	120.47	123.34
55	2x	54	5MU	O2-C2-N1	-2.72	119.17	122.79
1	1A	1942	5MC	C5-C4-N3	-2.70	118.76	121.67
54	1w	39	PSU	O2-C2-N1	-2.70	119.81	122.79
57	1y	32	PSU	C6-C5-C4	-2.70	116.31	118.20
1	1A	1962	5MC	C5-C4-N3	-2.68	118.78	121.67
32	2a	1404	5MC	C5-C4-N3	-2.68	118.78	121.67
32	2a	1407	5MC	C5-C4-N3	-2.65	118.81	121.67
32	1a	1518	MA6	C4-C5-N7	-2.65	106.64	109.40
54	2w	39	PSU	O2-C2-N1	-2.64	119.89	122.79
55	1x	8	4SU	C1'-N1-C2	2.62	122.31	117.57
54	2w	37	MIA	C2-N1-C6	2.61	121.86	117.19
32	1a	1400	5MC	C5-C4-N3	-2.60	118.86	121.67
54	2w	37	MIA	C4-C5-N7	-2.58	106.72	109.40
54	1w	8	4SU	C1'-N1-C2	2.57	122.22	117.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	2x	55	PSU	O2-C2-N1	-2.56	119.97	122.79
55	2x	8	4SU	O2-C2-N1	2.53	126.15	122.79
57	1y	8	4SU	C1'-N1-C2	2.52	122.14	117.57
1	2A	2251	OMG	CM2-O2'-C2'	-2.51	107.93	114.52
57	1y	54	5MU	C1'-N1-C2	2.51	122.11	117.57
1	2A	2552	OMU	C2'-C1'-N1	-2.50	109.37	114.22
1	2A	2251	OMG	C5-C6-N1	2.49	118.35	113.95
55	2x	32	5MC	C5-C4-N3	-2.49	118.99	121.67
32	2a	1402	4OC	C6-C5-C4	2.49	120.01	116.96
32	1a	1207	2MG	C8-N7-C5	2.48	107.72	102.99
32	1a	1402	4OC	C6-C5-C4	2.48	120.00	116.96
1	1A	2503	2MA	C8-N7-C5	2.48	107.71	102.99
32	1a	1404	5MC	O2-C2-N3	-2.47	118.31	122.33
1	2A	2503	2MA	C8-N7-C5	2.47	107.69	102.99
1	1A	1962	5MC	CM5-C5-C6	-2.45	119.57	122.85
57	1y	37	MIA	C4-C5-N7	-2.45	106.85	109.40
32	2a	967	5MC	C5-C4-N3	-2.43	119.05	121.67
1	2A	1942	5MC	C5-C4-N3	-2.43	119.05	121.67
1	2A	1939	5MU	C5M-C5-C4	2.43	121.44	118.77
32	1a	1498	UR3	C3U-N3-C4	2.43	121.36	117.89
1	1A	1917	PSU	C6-C5-C4	-2.42	116.50	118.20
1	1A	2503	2MA	C5-C6-N1	2.39	118.15	114.02
1	1A	2605	PSU	C5-C6-N1	-2.38	118.54	122.11
32	1a	966	M2G	C5-C6-N1	2.37	118.13	113.95
32	1a	967	5MC	C1'-N1-C6	-2.36	117.20	121.12
1	2A	2251	OMG	C8-N7-C5	2.36	107.48	102.99
32	1a	1402	4OC	O2-C2-N3	-2.35	118.50	122.33
54	2w	8	4SU	O2-C2-N1	-2.34	119.68	122.79
1	1A	2251	OMG	C5-C6-N1	2.33	118.06	113.95
1	2A	1915	5MU	O2-C2-N1	-2.32	119.70	122.79
1	1A	2251	OMG	C8-N7-C5	2.31	107.39	102.99
1	1A	1915	5MU	O2-C2-N1	-2.31	119.72	122.79
32	2a	1400	5MC	C5-C4-N3	-2.31	119.18	121.67
56	1z	1	FME	CA-N-CN	2.30	126.36	122.82
32	2a	1207	2MG	C8-N7-C5	2.30	107.37	102.99
43	1l	92	0TD	OD1-CG-CB	-2.27	117.68	122.44
1	1A	1920	OMC	O2-C2-N3	-2.27	118.64	122.33
57	2y	39	PSU	C5-C6-N1	-2.26	118.72	122.11
54	2w	37	MIA	N3-C2-N1	-2.26	122.83	126.98
32	1a	966	M2G	O6-C6-C5	-2.25	119.98	124.37
32	2a	966	M2G	C8-N7-C5	2.25	107.27	102.99
55	1x	8	4SU	O2-C2-N3	-2.23	117.34	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	2y	54	5MU	O2-C2-N3	-2.23	117.35	121.50
43	2l	92	0TD	OD1-CG-CB	-2.22	117.80	122.44
1	2A	1911	PSU	C5-C6-N1	-2.21	118.79	122.11
57	2y	46	G7M	C3'-C2'-C1'	2.21	104.30	100.98
55	1x	54	5MU	O2-C2-N1	-2.19	119.87	122.79
57	1y	54	5MU	C5-C6-N1	-2.19	121.09	123.34
54	2w	54	5MU	C5M-C5-C4	2.18	121.17	118.77
32	1a	1404	5MC	CM5-C5-C6	-2.17	119.95	122.85
54	1w	46	G7M	C3'-C2'-C1'	2.16	104.23	100.98
1	2A	2503	2MA	C5-C6-N1	2.14	117.71	114.02
32	2a	1498	UR3	C1'-N1-C2	2.14	120.60	116.99
32	1a	966	M2G	C8-N7-C5	2.14	107.06	102.99
57	2y	55	PSU	C6-C5-C4	-2.14	116.70	118.20
1	1A	2552	OMU	O4-C4-C5	-2.13	121.42	125.16
32	2a	1498	UR3	C3U-N3-C2	2.12	121.03	117.31
55	2x	8	4SU	O2-C2-N3	-2.12	117.55	121.50
1	1A	1942	5MC	O2-C2-N3	-2.12	118.89	122.33
55	2x	76	8AN	O2'-C2'-C3'	2.12	116.98	111.47
1	1A	1920	OMC	C1'-N1-C2	2.12	123.14	118.42
32	1a	967	5MC	C5-C4-N3	-2.11	119.39	121.67
54	1w	32	PSU	C6-C5-C4	-2.10	116.73	118.20
55	1x	32	5MC	O2-C2-N3	-2.08	118.96	122.33
1	2A	1962	5MC	C5-C4-N3	-2.08	119.44	121.67
1	1A	1915	5MU	C5M-C5-C4	2.07	121.05	118.77
1	2A	1939	5MU	C5M-C5-C6	-2.05	120.11	122.85
32	2a	1400	5MC	CM5-C5-C6	-2.04	120.12	122.85
54	1w	54	5MU	O2-C2-N1	-2.04	120.08	122.79
55	2x	32	5MC	O2-C2-N3	-2.04	119.02	122.33
55	2x	32	5MC	CM5-C5-C6	-2.04	120.13	122.85
32	2a	966	M2G	C5-C6-N1	2.04	117.55	113.95
32	2a	966	M2G	N1-C2-N2	-2.03	116.31	118.04
57	2y	8	4SU	O2-C2-N1	-2.02	120.10	122.79
55	1x	8	4SU	C4-N3-C2	2.01	129.29	127.34
55	2x	8	4SU	S4-C4-N3	-2.00	118.24	120.21

There are no chirality outliers.

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1A	2251	OMG	C1'-C2'-O2'-CM2
32	1a	1519	MA6	O4'-C4'-C5'-O5'
55	1x	76	8AN	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
57	1y	46	G7M	C4'-C5'-O5'-P
55	2x	76	8AN	C3'-C4'-C5'-O5'
57	2y	54	5MU	C3'-C4'-C5'-O5'
57	2y	54	5MU	O4'-C4'-C5'-O5'
54	1w	37	MIA	C12-C13-C14-C15
54	1w	37	MIA	C12-C13-C14-C16
54	2w	37	MIA	C5-C6-N6-C12
54	2w	37	MIA	N1-C6-N6-C12
56	1z	1	FME	O1-CN-N-CA
56	1z	1	FME	N-CA-CB-CG
56	1z	1	FME	C-CA-CB-CG
56	1z	1	FME	O-C-CA-CB
56	2z	1	FME	O1-CN-N-CA
56	2z	1	FME	CA-CB-CG-SD
32	1a	1519	MA6	C3'-C4'-C5'-O5'
32	2a	1519	MA6	O4'-C4'-C5'-O5'
55	2x	76	8AN	O4'-C4'-C5'-O5'
54	2w	32	PSU	C3'-C4'-C5'-O5'
54	2w	32	PSU	O4'-C4'-C5'-O5'
55	1x	76	8AN	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
32	2a	527	G7M	C3'-C4'-C5'-O5'
32	1a	527	G7M	C3'-C4'-C5'-O5'
54	2w	46	G7M	C4'-C5'-O5'-P
57	2y	46	G7M	O4'-C4'-C5'-O5'
54	2w	76	F3N	N-CA-CB-CG
54	1w	46	G7M	C4'-C5'-O5'-P
32	2a	527	G7M	O4'-C4'-C5'-O5'
57	2y	46	G7M	C3'-C4'-C5'-O5'
32	1a	1519	MA6	C4'-C5'-O5'-P
43	2l	92	0TD	CG-CB-SB-CSB
32	2a	527	G7M	C4'-C5'-O5'-P
57	2y	8	4SU	C4'-C5'-O5'-P
32	1a	1400	5MC	O4'-C4'-C5'-O5'
55	2x	76	8AN	C4'-C5'-O5'-P
32	1a	527	G7M	O4'-C4'-C5'-O5'
55	1x	76	8AN	C4'-C5'-O5'-P
57	1y	37	MIA	C3'-C4'-C5'-O5'
54	2w	76	F3N	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C4'-C5'-O5'-P
1	1A	2503	2MA	C4'-C5'-O5'-P
54	1w	37	MIA	N6-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
57	1y	32	PSU	O4'-C1'-C5-C4
57	1y	55	PSU	O4'-C1'-C5-C4
32	1a	527	G7M	C4'-C5'-O5'-P
43	2l	92	0TD	CA-CB-SB-CSB
54	2w	76	F3N	C-CA-CB-CG
32	1a	1400	5MC	C3'-C4'-C5'-O5'
57	2y	37	MIA	C3'-C4'-C5'-O5'
56	2z	1	FME	N-CA-CB-CG
43	1l	92	0TD	CG-CB-SB-CSB
57	1y	55	PSU	O4'-C1'-C5-C6
57	2y	55	PSU	O4'-C1'-C5-C6
1	1A	2503	2MA	O4'-C4'-C5'-O5'
57	1y	46	G7M	C3'-C4'-C5'-O5'
1	1A	1920	OMC	C2'-C1'-N1-C2
54	1w	37	MIA	N3-C2-S10-C11
1	2A	2503	2MA	O4'-C4'-C5'-O5'

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 2739 ligands modelled in this entry, 2737 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	304	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	304	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1A	2860/2915 (98%)	1.33	189 (6%) 18 23	19, 35, 83, 91	0
1	2A	2789/2915 (95%)	1.23	209 (7%) 14 19	31, 52, 81, 93	0
2	1B	120/121 (99%)	0.85	0 100 100	31, 47, 59, 77	0
2	2B	120/121 (99%)	0.95	8 (6%) 17 23	55, 66, 73, 80	0
3	1D	275/276 (99%)	1.05	10 (3%) 42 49	20, 36, 49, 69	0
3	2D	275/276 (99%)	1.33	32 (11%) 4 6	30, 46, 59, 69	0
4	1E	204/206 (99%)	1.15	19 (9%) 8 11	19, 39, 57, 67	0
4	2E	204/206 (99%)	0.95	15 (7%) 14 19	32, 53, 64, 73	0
5	1F	202/210 (96%)	0.97	10 (4%) 28 35	20, 40, 61, 73	0
5	2F	202/210 (96%)	1.06	19 (9%) 8 11	32, 61, 71, 76	0
6	1G	181/182 (99%)	0.82	7 (3%) 39 46	42, 54, 67, 78	0
6	2G	181/182 (99%)	1.21	30 (16%) 1 2	57, 68, 75, 81	0
7	1H	174/180 (96%)	0.93	10 (5%) 23 30	36, 52, 61, 66	0
7	2H	174/180 (96%)	2.86	120 (68%) 0 0	62, 71, 77, 80	0
8	1I	146/148 (98%)	0.90	17 (11%) 4 6	45, 66, 73, 77	0
8	2I	146/148 (98%)	1.49	42 (28%) 0 0	54, 70, 79, 83	0
9	1N	140/140 (100%)	1.30	20 (14%) 2 3	24, 38, 56, 70	0
9	2N	140/140 (100%)	1.27	23 (16%) 1 2	42, 57, 69, 71	0
10	1O	122/122 (100%)	0.99	4 (3%) 46 53	26, 38, 53, 58	0
10	2O	122/122 (100%)	0.96	5 (4%) 37 44	40, 52, 63, 71	0
11	1P	149/150 (99%)	0.93	7 (4%) 31 38	20, 43, 62, 67	0
11	2P	149/150 (99%)	1.42	36 (24%) 0 0	36, 60, 71, 75	0
12	1Q	141/141 (100%)	1.02	7 (4%) 28 35	23, 39, 53, 65	0
12	2Q	141/141 (100%)	1.59	43 (30%) 0 0	38, 57, 65, 70	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	1.02	6 (5%) 28 35	25, 35, 44, 54	0
13	2R	118/118 (100%)	0.91	9 (7%) 13 18	38, 49, 57, 61	0
14	1S	110/112 (98%)	0.87	3 (2%) 54 62	36, 47, 59, 62	0
14	2S	110/112 (98%)	1.25	18 (16%) 1 2	54, 63, 70, 73	0
15	1T	131/146 (89%)	0.86	8 (6%) 21 27	31, 42, 63, 73	0
15	2T	131/146 (89%)	0.97	11 (8%) 11 15	47, 55, 67, 73	0
16	1U	116/118 (98%)	1.15	8 (6%) 16 22	19, 29, 46, 57	0
16	2U	116/118 (98%)	1.10	14 (12%) 4 6	41, 54, 64, 67	0
17	1V	101/101 (100%)	1.07	9 (8%) 9 13	22, 38, 51, 60	0
17	2V	101/101 (100%)	1.06	10 (9%) 7 10	40, 61, 69, 74	0
18	1W	112/113 (99%)	1.33	17 (15%) 2 3	23, 32, 47, 75	0
18	2W	112/113 (99%)	1.01	6 (5%) 25 32	36, 46, 59, 77	0
19	1X	95/96 (98%)	1.28	13 (13%) 3 4	25, 36, 54, 73	0
19	2X	95/96 (98%)	1.13	8 (8%) 11 15	42, 54, 66, 70	0
20	1Y	107/110 (97%)	1.00	4 (3%) 41 48	34, 46, 60, 70	0
20	2Y	107/110 (97%)	1.14	13 (12%) 4 6	52, 64, 71, 77	0
21	1Z	154/206 (74%)	1.10	17 (11%) 5 7	38, 59, 73, 79	0
21	2Z	160/206 (77%)	2.15	70 (43%) 0 0	55, 71, 79, 83	0
22	10	83/85 (97%)	0.90	1 (1%) 79 83	27, 36, 47, 60	0
22	20	83/85 (97%)	1.45	16 (19%) 1 1	40, 54, 61, 71	0
23	11	97/98 (98%)	1.06	9 (9%) 8 11	28, 45, 65, 69	0
23	21	97/98 (98%)	1.35	18 (18%) 1 1	40, 55, 67, 73	0
24	12	70/72 (97%)	1.17	4 (5%) 23 30	35, 44, 57, 67	0
24	22	70/72 (97%)	0.88	5 (7%) 16 21	54, 62, 69, 71	0
25	13	59/60 (98%)	0.95	2 (3%) 45 52	25, 35, 52, 63	0
25	23	59/60 (98%)	1.59	20 (33%) 0 0	48, 55, 69, 72	0
26	14	69/71 (97%)	1.17	14 (20%) 1 1	47, 68, 77, 80	0
26	24	69/71 (97%)	1.69	17 (24%) 0 0	66, 73, 79, 82	0
27	15	59/60 (98%)	1.05	3 (5%) 28 35	21, 33, 51, 64	0
27	25	59/60 (98%)	0.93	4 (6%) 17 22	33, 46, 61, 71	0
28	16	53/54 (98%)	0.75	0 100 100	31, 39, 53, 59	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	1.12	10 (18%) 1 1	44, 54, 62, 65	0
29	17	48/49 (97%)	1.20	3 (6%) 20 25	18, 27, 51, 57	0
29	27	48/49 (97%)	1.44	7 (14%) 2 3	33, 41, 60, 68	0
30	18	64/65 (98%)	0.96	5 (7%) 13 17	27, 33, 39, 55	0
30	28	64/65 (98%)	1.43	16 (25%) 0 0	40, 50, 54, 59	0
31	19	37/37 (100%)	0.85	1 (2%) 54 62	28, 36, 49, 51	0
31	29	37/37 (100%)	2.19	20 (54%) 0 0	51, 58, 67, 69	0
32	1a	1488/1521 (97%)	1.25	163 (10%) 5 7	33, 58, 80, 90	0
32	2a	1491/1521 (98%)	1.29	195 (13%) 3 4	45, 67, 81, 91	0
33	1b	231/256 (90%)	1.12	30 (12%) 3 4	57, 68, 75, 81	0
33	2b	231/256 (90%)	1.66	79 (34%) 0 0	63, 72, 77, 83	0
34	1c	206/239 (86%)	1.49	49 (23%) 0 0	47, 61, 69, 75	0
34	2c	206/239 (86%)	1.93	88 (42%) 0 0	63, 71, 76, 81	0
35	1d	208/209 (99%)	1.25	43 (20%) 1 1	48, 59, 67, 72	0
35	2d	208/209 (99%)	1.27	39 (18%) 1 1	53, 65, 72, 79	0
36	1e	148/162 (91%)	1.28	28 (18%) 1 1	45, 56, 64, 70	0
36	2e	148/162 (91%)	1.55	42 (28%) 0 0	57, 66, 72, 78	0
37	1f	100/101 (99%)	0.66	4 (4%) 38 45	49, 58, 66, 68	0
37	2f	100/101 (99%)	0.96	5 (5%) 28 35	51, 61, 66, 69	0
38	1g	155/156 (99%)	1.34	34 (21%) 0 1	54, 62, 73, 78	0
38	2g	155/156 (99%)	1.76	46 (29%) 0 0	64, 70, 77, 80	0
39	1h	137/138 (99%)	1.01	16 (11%) 4 6	48, 59, 65, 69	0
39	2h	137/138 (99%)	1.46	31 (22%) 0 1	57, 67, 71, 75	0
40	1i	127/128 (99%)	1.84	49 (38%) 0 0	47, 66, 72, 76	0
40	2i	127/128 (99%)	2.79	81 (63%) 0 0	62, 72, 77, 79	0
41	1j	97/105 (92%)	1.54	29 (29%) 0 0	49, 65, 73, 79	0
41	2j	96/105 (91%)	2.36	53 (55%) 0 0	63, 73, 77, 79	0
42	1k	114/129 (88%)	1.19	17 (14%) 2 3	44, 61, 70, 75	0
42	2k	114/129 (88%)	1.20	13 (11%) 5 7	51, 65, 70, 74	0
43	1l	121/132 (91%)	1.11	15 (12%) 4 5	37, 47, 59, 62	0
43	2l	121/132 (91%)	1.28	22 (18%) 1 1	50, 58, 66, 69	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
44	1m	123/126 (97%)	1.29	24 (19%)	1	1	49, 61, 69, 78	0
44	2m	122/126 (96%)	1.49	31 (25%)	0	0	61, 70, 74, 77	0
45	1n	60/61 (98%)	1.86	24 (40%)	0	0	47, 56, 63, 65	0
45	2n	60/61 (98%)	3.14	47 (78%)	0	0	66, 71, 74, 76	0
46	1o	88/89 (98%)	0.98	9 (10%)	6	9	44, 55, 65, 71	0
46	2o	88/89 (98%)	1.32	18 (20%)	1	1	53, 63, 70, 72	0
47	1p	82/88 (93%)	1.73	28 (34%)	0	0	50, 61, 66, 69	0
47	2p	82/88 (93%)	1.19	10 (12%)	4	6	56, 63, 70, 74	0
48	1q	99/105 (94%)	1.46	23 (23%)	0	1	50, 60, 67, 70	0
48	2q	99/105 (94%)	1.57	35 (35%)	0	0	56, 64, 70, 72	0
49	1r	68/88 (77%)	0.84	6 (8%)	10	13	50, 58, 66, 68	0
49	2r	68/88 (77%)	0.99	4 (5%)	22	28	56, 62, 70, 75	0
50	1s	83/93 (89%)	1.49	20 (24%)	0	0	55, 63, 71, 74	0
50	2s	83/93 (89%)	1.92	36 (43%)	0	0	67, 72, 77, 79	0
51	1t	96/106 (90%)	2.45	51 (53%)	0	0	56, 62, 70, 74	0
51	2t	96/106 (90%)	1.72	31 (32%)	0	0	54, 63, 72, 76	0
52	1u	23/27 (85%)	2.54	14 (60%)	0	0	55, 59, 62, 66	0
52	2u	23/27 (85%)	2.67	18 (78%)	0	0	68, 70, 73, 74	0
53	1v	13/24 (54%)	2.40	6 (46%)	0	0	40, 47, 82, 85	0
53	2v	13/24 (54%)	4.07	10 (76%)	0	0	60, 80, 87, 89	0
54	1w	66/76 (86%)	1.84	19 (28%)	0	0	25, 74, 83, 87	0
54	2w	64/76 (84%)	2.15	24 (37%)	0	0	42, 79, 86, 88	0
55	1x	72/77 (93%)	1.18	5 (6%)	16	22	24, 57, 71, 81	0
55	2x	72/77 (93%)	1.10	6 (8%)	11	15	37, 67, 77, 82	0
56	1z	6/7 (85%)	6.94	4 (66%)	0	0	25, 35, 44, 63	0
56	2z	6/7 (85%)	6.70	3 (50%)	0	0	37, 40, 54, 67	0
57	1y	67/76 (88%)	5.52	67 (100%)	0	0	58, 85, 88, 89	0
57	2y	66/76 (86%)	5.67	66 (100%)	0	0	68, 88, 91, 92	0
All	All	20883/21762 (95%)	1.33	3111 (14%)	2	3	18, 57, 77, 93	0

All (3111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
56	1z	2	THR	20.9
56	2z	2	THR	17.3
57	2y	36	A	13.1
44	2m	124	PRO	12.8
44	1m	124	PRO	12.8
57	2y	29	G	11.5
54	2w	71	G	10.9
56	2z	4	SER	10.8
57	1y	35	A	10.7
1	1A	2145	C	10.6
57	1y	34	G	10.2
57	1y	36	A	10.1
53	2v	24	A	10.0
40	2i	14	VAL	10.0
1	2A	2127	G	9.8
38	2g	80	VAL	9.8
57	2y	34	G	9.7
1	1A	2146	C	9.6
57	2y	57	G	9.4
1	2A	2112	G	9.3
56	1z	3	HIS	9.0
44	1m	123	ALA	9.0
21	2Z	155	LEU	8.9
7	2H	35	VAL	8.9
1	2A	2146	C	8.8
1	1A	2131	G	8.7
7	2H	98	LEU	8.7
21	2Z	144	LEU	8.7
56	2z	3	HIS	8.7
57	1y	5	G	8.6
1	2A	2115	G	8.5
45	2n	38	GLY	8.5
1	1A	2160	G	8.5
40	2i	67	GLY	8.5
54	1w	70	G	8.5
57	2y	35	A	8.5
57	1y	19	G	8.4
1	2A	2161	C	8.4
57	2y	15	G	8.3
57	2y	19	G	8.2
1	1A	2140	C	8.1
1	2A	2117	A	8.1
34	2c	159	GLY	8.1

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Mol	Chain	Res	Type	RSRZ
1	1A	2115	G	8.1
1	2A	2160	G	8.1
1	1A	2147	G	8.1
1	2A	2162	G	8.1
57	1y	21	A	8.0
38	1g	81	GLY	7.9
1	2A	2145	C	7.9
57	1y	38	A	7.9
1	1A	2159	G	7.9
1	1A	2129	C	7.9
21	2Z	149	SER	7.8
44	2m	123	ALA	7.8
7	2H	24	VAL	7.8
8	2I	107	VAL	7.8
57	1y	24	G	7.7
57	2y	62	C	7.7
1	2A	2128	C	7.7
56	1z	4	SER	7.6
1	2A	2133	G	7.6
57	1y	1	G	7.6
1	2A	2147	G	7.6
32	2a	1030(A)	G	7.6
53	2v	22	U	7.6
51	1t	95	ALA	7.6
57	2y	31	A	7.5
1	2A	2123	G	7.5
1	2A	883	G	7.5
7	2H	105	LEU	7.5
26	24	50	VAL	7.4
1	1A	2141	G	7.4
1	2A	884	C	7.4
53	2v	12	A	7.4
57	2y	74	C	7.4
1	1A	2112	G	7.4
1	2A	2138	C	7.4
1	2A	2166	G	7.4
57	1y	58	A	7.4
1	2A	2159	G	7.4
26	24	51	ASP	7.4
1	1A	1096	A	7.3
32	2a	1030(B)	C	7.3
1	2A	2142	C	7.3

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Mol	Chain	Res	Type	RSRZ
1	2A	2168	G	7.3
1	2A	885	C	7.3
38	2g	82	GLY	7.2
1	1A	2178	C	7.2
1	2A	2139	C	7.2
1	2A	2181	G	7.2
57	1y	57	G	7.1
1	1A	2175	C	7.1
1	1A	2181	G	7.1
1	1A	2117	A	7.1
1	2A	2129	C	7.1
1	2A	2116	G	7.0
1	2A	2114	A	7.0
38	2g	81	GLY	6.9
57	2y	33	U	6.9
1	2A	2113	U	6.9
38	1g	79	ARG	6.9
1	2A	2125	G	6.9
1	1A	2161	C	6.9
57	1y	2	C	6.9
26	24	49	PHE	6.9
1	1A	2133	G	6.9
26	24	63	TYR	6.9
1	2A	2158	A	6.9
1	1A	2110	G	6.9
57	2y	14	A	6.8
57	2y	26	A	6.8
41	2j	38	ILE	6.8
57	1y	53	G	6.8
57	2y	1	G	6.8
40	2i	65	VAL	6.7
1	2A	2110	G	6.7
1	2A	888	C	6.7
1	2A	2143	C	6.7
57	2y	28	G	6.6
34	2c	157	ILE	6.6
32	1a	1036	G	6.6
1	2A	2170	A	6.6
1	1A	2116	G	6.6
1	1A	2188	C	6.6
1	2A	2141	G	6.5
1	1A	2111	C	6.5

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Mol	Chain	Res	Type	RSRZ
33	2b	165	VAL	6.5
57	1y	13	C	6.5
57	1y	56	C	6.5
1	1A	2114	A	6.5
57	1y	27	G	6.5
41	1j	18	ALA	6.5
1	1A	2174	C	6.5
1	1A	2162	G	6.5
32	2a	1034	G	6.5
1	1A	2168	G	6.5
1	1A	2170	A	6.5
53	1v	12	A	6.4
57	2y	21	A	6.4
57	2y	63	G	6.4
1	1A	2158	A	6.4
54	2w	72	C	6.4
57	2y	48	C	6.4
1	2A	2120	G	6.4
57	1y	70	G	6.4
53	1v	13	A	6.4
57	1y	75	C	6.4
57	2y	25	C	6.4
1	2A	2182	G	6.3
41	2j	74	ILE	6.3
32	2a	1033	G	6.3
57	2y	75	C	6.3
1	2A	2149	G	6.3
57	1y	30	G	6.3
54	2w	70	G	6.3
32	2a	1031	G	6.3
57	2y	18	G	6.3
18	2W	112	GLY	6.3
1	2A	2167	U	6.2
1	2A	2126	A	6.2
32	2a	1030	C	6.2
57	1y	49	C	6.2
1	2A	2111	C	6.2
38	1g	156	TRP	6.2
1	1A	1076	C	6.2
34	2c	87	LEU	6.2
1	1A	884	C	6.2
1	1A	2108	C	6.2

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Mol	Chain	Res	Type	RSRZ
1	2A	2174	C	6.2
1	1A	2123	G	6.2
32	1a	1030(A)	G	6.2
57	2y	5	G	6.2
21	2Z	170	THR	6.2
1	2A	2104	G	6.1
1	1A	1095	A	6.1
45	2n	25	VAL	6.1
57	2y	56	C	6.1
57	2y	53	G	6.1
41	2j	98	ILE	6.1
32	1a	1029	C	6.1
51	1t	43	LEU	6.1
1	2A	2155	G	6.1
57	1y	29	G	6.1
51	1t	59	ALA	6.0
7	2H	99	VAL	6.0
38	2g	154	TYR	6.0
32	1a	1001	A	6.0
1	2A	2121	G	6.0
57	1y	71	G	6.0
1	1A	887	A	6.0
32	1a	1001(A)	G	6.0
40	1i	117	HIS	6.0
1	1A	1509	C	6.0
1	1A	2142	C	6.0
21	2Z	153	SER	5.9
32	2a	1001(A)	G	5.9
7	2H	44	VAL	5.9
57	1y	31	A	5.9
7	2H	128	PRO	5.9
1	1A	2165	G	5.9
40	2i	109	VAL	5.9
38	2g	40	ALA	5.9
40	2i	5	TYR	5.9
1	1A	2154	G	5.9
47	1p	60	LEU	5.9
57	1y	23	A	5.9
1	2A	2175	C	5.9
1	1A	2120	G	5.9
57	2y	30	G	5.9
57	1y	20	U	5.9

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Mol	Chain	Res	Type	RSRZ
7	2H	72	ILE	5.9
47	1p	19	ILE	5.9
8	2I	100	ALA	5.9
1	1A	2164	C	5.9
57	2y	10	G	5.9
57	2y	52	G	5.9
34	2c	198	VAL	5.8
26	24	59	PHE	5.8
32	2a	1036	G	5.8
34	2c	124	ILE	5.8
50	1s	72	GLY	5.8
41	2j	72	VAL	5.8
1	2A	2169	A	5.8
57	2y	38	A	5.8
38	2g	156	TRP	5.8
57	2y	61	C	5.8
1	2A	2188	C	5.8
1	2A	2165	G	5.8
51	1t	62	LEU	5.8
1	2A	2144	U	5.8
21	2Z	139	VAL	5.8
1	2A	892	G	5.8
54	1w	71	G	5.8
1	1A	896	A	5.7
51	1t	100	ILE	5.7
41	2j	44	VAL	5.7
1	1A	2113	U	5.7
1	1A	2135	A	5.7
1	1A	2169	A	5.7
1	2A	2179	C	5.7
32	2a	1027	C	5.7
51	1t	47	GLY	5.7
57	1y	69	G	5.6
1	1A	2179	C	5.6
32	1a	1028	C	5.6
57	1y	14	A	5.6
51	1t	13	LEU	5.6
40	2i	90	PRO	5.6
57	1y	61	C	5.6
38	2g	79	ARG	5.6
57	2y	64	A	5.6
40	2i	102	LEU	5.6

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Mol	Chain	Res	Type	RSRZ
1	1A	2127	G	5.6
34	2c	39	ILE	5.6
45	2n	24	CYS	5.6
32	1a	1030(B)	C	5.6
45	2n	42	ILE	5.6
1	2A	2154	G	5.6
1	1A	2144	U	5.5
57	1y	63	G	5.5
1	2A	2164	C	5.5
1	2A	2100	G	5.5
32	1a	1003	G	5.5
23	1l	2	SER	5.5
45	2n	34	TYR	5.5
57	1y	64	A	5.5
1	1A	2148	G	5.5
32	2a	1032	G	5.5
51	2t	41	ILE	5.5
41	2j	40	LEU	5.5
1	2A	2106	G	5.5
1	1A	2130	U	5.5
57	1y	74	C	5.5
54	2w	4	C	5.4
36	2e	32	VAL	5.4
57	2y	23	A	5.4
1	1A	2128	C	5.4
7	2H	25	LYS	5.4
1	1A	897	C	5.4
51	1t	9	ASN	5.4
32	1a	1286	A	5.4
32	2a	1035	A	5.4
1	1A	2166	G	5.4
1	2A	2148	G	5.4
33	1b	229	VAL	5.4
21	2Z	106	GLY	5.3
48	2q	33	GLY	5.3
57	1y	52	G	5.3
21	2Z	145	GLU	5.3
57	1y	25	C	5.3
57	2y	2	C	5.3
44	2m	120	LYS	5.3
21	2Z	148	ASP	5.3
12	2Q	114	ALA	5.3

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Mol	Chain	Res	Type	RSRZ
32	2a	1002	G	5.3
57	1y	10	G	5.3
1	1A	2143	C	5.3
34	1c	196	LEU	5.3
3	2D	2	ALA	5.3
50	2s	31	ILE	5.3
1	2A	887	A	5.3
1	1A	892	G	5.3
57	1y	3	C	5.3
57	1y	62	C	5.3
57	1y	28	G	5.3
7	2H	102	ALA	5.3
40	2i	72	GLY	5.3
57	2y	43	C	5.2
57	2y	65	G	5.2
1	1A	1064	C	5.2
1	1A	2182	G	5.2
7	2H	73	ALA	5.2
1	1A	2109	U	5.2
51	1t	22	ARG	5.2
33	2b	34	ALA	5.2
17	2V	72	VAL	5.2
38	1g	80	VAL	5.2
57	1y	33	U	5.2
57	2y	27	G	5.2
23	2l	2	SER	5.2
35	1d	138	TYR	5.2
1	2A	2177	C	5.2
54	2w	31	A	5.2
1	1A	885	C	5.1
57	2y	4	C	5.1
45	2n	13	THR	5.1
48	1q	36	ILE	5.1
57	2y	24	G	5.1
57	1y	4	C	5.1
1	1A	2180	U	5.1
45	2n	37	PHE	5.1
7	2H	36	PRO	5.1
1	2A	886	C	5.1
33	2b	187	LEU	5.1
45	2n	39	LEU	5.1
32	1a	1257	U	5.1

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Mol	Chain	Res	Type	RSRZ
57	1y	15	G	5.1
57	1y	18	G	5.1
28	26	52	VAL	5.1
32	1a	999	C	5.1
21	2Z	141	VAL	5.1
57	2y	12	U	5.1
50	2s	63	THR	5.0
32	1a	1031	G	5.0
40	2i	74	ILE	5.0
50	2s	49	ILE	5.0
1	1A	888	C	5.0
1	2A	2163	C	5.0
41	1j	36	GLY	5.0
51	1t	84	LEU	5.0
57	2y	58	A	5.0
1	1A	2101	G	5.0
1	2A	2152	G	5.0
32	2a	1030(C)	G	5.0
40	2i	9	ARG	5.0
40	2i	62	TYR	5.0
57	1y	48	C	5.0
1	2A	2157	G	5.0
34	1c	15	THR	5.0
21	2Z	151	HIS	5.0
1	2A	229	A	5.0
7	2H	29	PRO	4.9
40	1i	14	VAL	4.9
50	2s	67	VAL	4.9
57	1y	67	C	4.9
32	2a	1250	A	4.9
40	2i	7	THR	4.9
40	2i	125	TYR	4.9
32	1a	1032	G	4.9
7	2H	100	GLY	4.9
53	2v	13	A	4.9
57	2y	73	A	4.9
7	2H	19	VAL	4.9
47	1p	78	GLY	4.9
1	2A	2802	G	4.9
57	2y	44	G	4.9
6	2G	29	TRP	4.9
34	2c	100	ALA	4.9

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Mol	Chain	Res	Type	RSRZ
47	1p	32	TYR	4.9
51	1t	72	LEU	4.9
33	1b	232	PRO	4.9
1	1A	229	A	4.9
7	2H	107	VAL	4.9
40	2i	43	ALA	4.8
1	2A	2183	C	4.8
57	2y	41	C	4.8
40	2i	126	SER	4.8
52	2u	13	ILE	4.8
1	2A	896	A	4.8
51	1t	55	ILE	4.8
1	1A	2104	G	4.8
7	2H	96	ALA	4.8
32	2a	1287	A	4.8
1	2A	897	C	4.8
32	2a	1039	C	4.8
33	2b	215	LEU	4.8
42	2k	25	TYR	4.8
44	2m	87	TYR	4.8
5	2F	15	SER	4.8
57	2y	6	G	4.8
57	2y	71	G	4.8
1	1A	886	C	4.8
1	2A	2108	C	4.8
4	1E	195	LEU	4.8
1	2A	2156	G	4.7
32	2a	1021	G	4.7
7	2H	34	GLU	4.7
40	2i	36	TYR	4.7
52	1u	14	TRP	4.7
1	1A	890	A	4.7
1	1A	2105	C	4.7
57	2y	68	C	4.7
34	2c	145	GLY	4.7
1	1A	1084	A	4.7
57	1y	65	G	4.7
50	2s	80	TYR	4.7
38	2g	31	MET	4.7
1	1A	889	C	4.7
53	1v	14	A	4.7
1	2A	881	G	4.7

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Mol	Chain	Res	Type	RSRZ
32	1a	1532	U	4.7
34	1c	158	GLY	4.7
33	2b	33	TYR	4.7
38	2g	23	VAL	4.7
51	1t	18	GLN	4.7
48	1q	28	PRO	4.7
1	2A	2105	C	4.7
57	1y	68	C	4.7
1	1A	2106	G	4.7
44	2m	68	GLY	4.7
40	2i	106	ALA	4.7
7	2H	45	VAL	4.6
1	1A	2132	U	4.6
40	2i	27	THR	4.6
45	1n	2	ALA	4.6
53	2v	23	A	4.6
32	2a	80	G	4.6
7	2H	52	VAL	4.6
48	1q	31	LEU	4.6
1	2A	2107	C	4.6
54	2w	73	A	4.6
1	2A	1170	G	4.6
32	1a	1030(C)	G	4.6
1	2A	2122	U	4.6
57	2y	13	C	4.6
1	1A	2149	G	4.6
45	2n	43	CYS	4.6
12	2Q	109	VAL	4.6
32	2a	1026	G	4.6
57	2y	22	G	4.6
21	2Z	150	LEU	4.6
7	2H	6	ARG	4.6
39	2h	58	TYR	4.6
41	2j	88	LEU	4.6
38	2g	83	ALA	4.5
51	1t	44	ALA	4.5
1	1A	1075	C	4.5
33	1b	227	GLY	4.5
36	2e	10	MET	4.5
1	1A	1057	A	4.5
1	1A	2121	G	4.5
26	14	54	GLY	4.5

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Mol	Chain	Res	Type	RSRZ
1	2A	2109	U	4.5
32	2a	1150	U	4.5
33	2b	232	PRO	4.5
32	1a	1531	A	4.5
43	2l	39	VAL	4.5
35	1d	120	LEU	4.5
51	2t	13	LEU	4.5
1	1A	1059	G	4.5
32	2a	1202	G	4.5
54	1w	44	G	4.5
57	1y	22	G	4.5
33	2b	17	PHE	4.5
7	2H	16	SER	4.5
7	2H	141	VAL	4.5
41	2j	65	LEU	4.5
36	2e	11	ILE	4.5
1	2A	898	C	4.5
1	2A	2103	C	4.5
1	2A	2134	A	4.5
32	2a	1030(D)	A	4.5
45	1n	25	VAL	4.5
1	1A	1063	G	4.5
1	2A	1026	U	4.5
57	2y	51	U	4.5
50	2s	84	GLY	4.5
1	1A	2187	G	4.5
1	2A	2178	C	4.4
33	2b	48	MET	4.4
50	2s	79	THR	4.4
41	2j	34	VAL	4.4
41	2j	19	SER	4.4
57	1y	6	G	4.4
1	1A	1072	C	4.4
33	2b	216	SER	4.4
38	1g	154	TYR	4.4
50	2s	57	HIS	4.4
7	2H	165	ALA	4.4
41	1j	16	LEU	4.4
7	2H	113	VAL	4.4
51	2t	26	ASN	4.4
1	2A	2135	A	4.4
45	2n	61	TRP	4.4

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Mol	Chain	Res	Type	RSRZ
45	2n	55	GLY	4.4
52	1u	2	GLY	4.4
32	2a	1286	A	4.4
57	2y	76	A	4.4
57	1y	72	C	4.4
1	1A	2157	G	4.4
32	2a	1024	G	4.4
7	2H	115	VAL	4.4
43	2l	55	VAL	4.4
1	2A	652(B)	A	4.4
57	1y	73	A	4.4
21	2Z	159	PRO	4.4
32	1a	1027	C	4.4
12	2Q	37	LEU	4.3
1	2A	2172	U	4.3
26	24	45	GLY	4.3
33	2b	44	LEU	4.3
51	1t	36	LEU	4.3
57	1y	44	G	4.3
49	2r	24	ALA	4.3
34	2c	81	GLY	4.3
32	1a	171	A	4.3
40	2i	17	VAL	4.3
1	2A	2137	C	4.3
36	2e	90	VAL	4.3
1	2A	2124	G	4.3
1	2A	2189	U	4.3
21	2Z	154	ASP	4.3
43	2l	64	TYR	4.3
1	1A	2107	C	4.3
1	2A	894	C	4.3
1	2A	2140	C	4.3
33	2b	98	LEU	4.3
57	2y	72	C	4.3
44	2m	84	ILE	4.3
57	2y	70	G	4.3
1	2A	2173	A	4.3
7	2H	8	PRO	4.2
52	2u	23	PRO	4.2
1	1A	2100	G	4.2
32	1a	162	A	4.2
57	2y	3	C	4.2

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Mol	Chain	Res	Type	RSRZ
7	2H	37	VAL	4.2
33	2b	112	VAL	4.2
41	1j	38	ILE	4.2
33	2b	28	PHE	4.2
45	2n	36	PHE	4.2
1	2A	1041	C	4.2
1	2A	1042	G	4.2
1	2A	1114	G	4.2
1	2A	2190	G	4.2
45	2n	11	LYS	4.2
14	2S	20	ARG	4.2
48	1q	27	PHE	4.2
38	2g	16	LEU	4.2
41	2j	24	VAL	4.2
6	2G	20	ILE	4.2
52	2u	14	TRP	4.2
45	2n	35	ARG	4.2
1	1A	2171	A	4.2
32	2a	1007	C	4.2
34	2c	92	ALA	4.2
41	2j	96	ILE	4.2
51	1t	45	GLN	4.2
31	29	12	ASP	4.2
1	2A	1533	G	4.2
52	1u	8	THR	4.2
7	2H	112	PRO	4.2
51	2t	72	LEU	4.2
34	1c	193	TYR	4.2
57	2y	49	C	4.2
57	1y	50	U	4.2
57	2y	47	U	4.2
45	1n	51	GLY	4.2
32	2a	216	G	4.1
32	1a	1446	U	4.1
32	2a	1157	A	4.1
53	2v	14	A	4.1
14	2S	5	THR	4.1
32	1a	1002	G	4.1
32	1a	1021	G	4.1
32	1a	1041	A	4.1
32	2a	1531	A	4.1
3	1D	2	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
36	2e	104	ALA	4.1
50	2s	50	ALA	4.1
57	2y	45	U	4.1
40	2i	57	GLY	4.1
1	2A	1509	C	4.1
1	2A	2319	G	4.1
32	1a	1026	G	4.1
32	2a	1116	C	4.1
57	1y	42	C	4.1
34	2c	86	VAL	4.1
40	1i	121	ARG	4.1
52	2u	21	TYR	4.1
21	2Z	147	GLY	4.1
1	1A	2103	C	4.1
21	2Z	100	VAL	4.1
34	2c	160	ALA	4.1
39	2h	134	ILE	4.1
34	2c	158	GLY	4.1
22	20	45	PHE	4.1
7	2H	26	VAL	4.1
32	2a	1018	C	4.1
40	1i	76	ALA	4.1
32	1a	1023	G	4.1
32	1a	1024	G	4.1
1	1A	2126	A	4.1
1	2A	2176	A	4.1
21	2Z	171	ILE	4.1
32	1a	1030(D)	A	4.1
31	29	37	GLY	4.1
45	2n	3	ARG	4.1
45	2n	29	ARG	4.1
19	2X	92	LEU	4.1
41	2j	47	PHE	4.1
1	1A	2138	C	4.0
33	2b	75	LYS	4.0
45	2n	26	ARG	4.0
1	1A	1094	U	4.0
33	1b	118	LEU	4.0
51	1t	38	LYS	4.0
30	28	18	ALA	4.0
40	2i	82	ALA	4.0
40	2i	66	ARG	4.0

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Mol	Chain	Res	Type	RSRZ
52	2u	22	ARG	4.0
1	1A	2163	C	4.0
26	14	56	VAL	4.0
43	2l	18	VAL	4.0
57	2y	67	C	4.0
7	2H	92	ILE	4.0
34	2c	8	ILE	4.0
51	1t	69	GLY	4.0
6	2G	49	ASP	4.0
7	2H	51	ARG	4.0
7	2H	20	ALA	4.0
33	1b	228	GLY	4.0
54	1w	72	C	4.0
57	2y	11	C	4.0
7	2H	148	ILE	4.0
14	2S	35	ILE	4.0
40	2i	63	ILE	4.0
6	2G	76	SER	4.0
40	1i	126	SER	4.0
1	2A	2119	A	4.0
1	2A	2151	G	4.0
32	1a	1033	G	4.0
51	1t	64	ASP	4.0
38	2g	32	ARG	4.0
41	2j	26	ALA	4.0
1	1A	2136	C	4.0
32	1a	1030	C	4.0
1	1A	1068	G	4.0
32	2a	1023	G	4.0
1	1A	2118	U	4.0
4	2E	52	LEU	4.0
50	1s	71	LEU	4.0
51	1t	40	ALA	4.0
12	2Q	6	ARG	4.0
29	27	46	VAL	4.0
32	2a	91	C	4.0
44	1m	117	VAL	4.0
40	2i	81	ILE	4.0
57	1y	60	U	4.0
1	1A	2184	G	4.0
7	2H	103	LEU	4.0
31	29	30	PRO	4.0

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Mol	Chain	Res	Type	RSRZ
7	2H	121	ILE	3.9
40	2i	4	TYR	3.9
1	1A	1069	A	3.9
43	2l	93	LEU	3.9
1	1A	1087	G	3.9
40	1i	84	ALA	3.9
21	2Z	69	THR	3.9
57	1y	47	U	3.9
36	2e	34	VAL	3.9
33	2b	51	LEU	3.9
1	1A	2134	A	3.9
1	1A	2190	G	3.9
1	2A	2118	U	3.9
1	2A	2184	G	3.9
57	1y	51	U	3.9
34	1c	66	VAL	3.9
12	2Q	19	GLY	3.9
1	2A	2180	U	3.9
34	2c	204	LEU	3.9
36	1e	132	ALA	3.9
50	2s	30	LEU	3.9
57	2y	50	U	3.9
54	1w	14	A	3.9
36	2e	16	THR	3.9
1	1A	2125	G	3.9
1	2A	889	C	3.9
57	1y	40	C	3.9
57	2y	42	C	3.9
45	2n	12	ARG	3.9
51	1t	83	ARG	3.9
1	1A	2151	G	3.9
54	2w	44	G	3.9
52	2u	2	GLY	3.9
1	1A	893	C	3.9
20	2Y	1	MET	3.9
12	2Q	20	ALA	3.9
26	24	66	SER	3.9
38	2g	4	ARG	3.9
39	2h	120	THR	3.9
43	1l	61	THR	3.9
1	1A	1070	A	3.9
1	1A	2167	U	3.9

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Mol	Chain	Res	Type	RSRZ
1	2A	2101	G	3.9
33	2b	127	ILE	3.9
47	2p	51	VAL	3.9
12	2Q	113	GLN	3.9
32	2a	1008	C	3.9
57	2y	40	C	3.9
32	2a	1257	U	3.8
1	1A	1099	G	3.8
25	23	54	VAL	3.8
32	2a	1029	C	3.8
1	1A	2189	U	3.8
7	2H	54	ARG	3.8
1	2A	2171	A	3.8
34	2c	134	ILE	3.8
40	1i	106	ALA	3.8
33	2b	11	LEU	3.8
52	1u	18	TYR	3.8
34	2c	109	PRO	3.8
1	1A	1060	U	3.8
32	2a	204	U	3.8
1	2A	2136	C	3.8
1	2A	2186	G	3.8
41	2j	29	ARG	3.8
40	1i	31	GLN	3.8
53	2v	21	C	3.8
34	2c	193	TYR	3.8
36	2e	146	ALA	3.8
47	1p	1	MET	3.8
1	1A	879	G	3.8
1	1A	2185	C	3.8
32	1a	1037	C	3.8
32	1a	841	U	3.8
32	2a	1532	U	3.8
5	1F	16	GLY	3.8
57	1y	26	A	3.8
7	2H	17	VAL	3.8
45	2n	2	ALA	3.8
48	2q	9	VAL	3.8
50	1s	31	ILE	3.8
1	1A	2139	C	3.8
45	2n	44	LEU	3.8
38	2g	78	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
40	2i	10	ARG	3.8
40	2i	114	TYR	3.8
40	2i	115	GLY	3.7
11	2P	127	ALA	3.7
21	2Z	57	ILE	3.7
57	2y	66	U	3.7
1	1A	2177	C	3.7
12	1Q	59	ARG	3.7
40	2i	19	LEU	3.7
48	2q	80	GLY	3.7
41	2j	11	PHE	3.7
40	2i	15	ALA	3.7
7	2H	43	VAL	3.7
40	2i	108	VAL	3.7
51	2t	16	HIS	3.7
32	2a	1028	C	3.7
32	1a	1034	G	3.7
1	1A	2122	U	3.7
34	1c	180	ALA	3.7
41	2j	27	ALA	3.7
1	1A	2119	A	3.7
50	2s	71	LEU	3.7
1	2A	2804	C	3.7
44	2m	64	TRP	3.7
54	1w	69	G	3.7
50	1s	39	THR	3.7
26	14	66	SER	3.7
43	1l	18	VAL	3.7
52	1u	13	ILE	3.7
23	2l	68	PRO	3.7
7	2H	31	GLY	3.7
57	1y	7	A	3.7
1	1A	1092	C	3.7
57	1y	11	C	3.7
34	2c	186	PHE	3.7
40	2i	71	SER	3.7
36	1e	10	MET	3.7
36	2e	13	ILE	3.7
38	2g	27	ILE	3.7
44	2m	78	ILE	3.7
7	2H	67	LEU	3.7
1	2A	652(T)	C	3.7

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Mol	Chain	Res	Type	RSRZ
1	2A	1040	C	3.7
21	2Z	93	ASP	3.7
7	2H	106	THR	3.7
32	2a	1385	G	3.7
34	2c	49	SER	3.7
21	2Z	22	GLY	3.7
33	2b	228	GLY	3.7
39	2h	94	TYR	3.7
21	2Z	58	VAL	3.7
25	23	47	VAL	3.7
38	2g	9	VAL	3.7
39	1h	6	ILE	3.7
40	1i	19	LEU	3.6
32	1a	1025	U	3.6
5	1F	21	ALA	3.6
26	24	52	THR	3.6
33	1b	120	ALA	3.6
1	1A	1093	G	3.6
7	2H	40	GLU	3.6
32	2a	1003	G	3.6
44	2m	69	GLU	3.6
47	1p	66	PRO	3.6
9	2N	72	TYR	3.6
12	2Q	32	TYR	3.6
36	2e	105	VAL	3.6
40	1i	81	ILE	3.6
34	2c	178	LEU	3.6
1	1A	1175	U	3.6
57	1y	59	U	3.6
32	1a	1035	A	3.6
33	2b	227	GLY	3.6
40	2i	49	PRO	3.6
11	2P	91	PHE	3.6
1	1A	1058	G	3.6
7	2H	76	VAL	3.6
11	2P	101	VAL	3.6
21	2Z	1	MET	3.6
32	1a	204	U	3.6
32	2a	1040	U	3.6
33	2b	81	VAL	3.6
38	1g	85	TYR	3.6
21	2Z	51	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
45	2n	14	PRO	3.6
1	1A	271(K)	U	3.6
1	2A	1039	G	3.6
1	2A	2191	G	3.6
8	2I	1	MET	3.6
6	1G	146	TYR	3.6
34	2c	18	TRP	3.6
21	2Z	156	LYS	3.6
32	2a	1041	A	3.6
8	2I	11	ASN	3.6
40	2i	121	ARG	3.6
21	2Z	50	GLN	3.6
1	2A	652(U)	G	3.6
30	28	23	VAL	3.6
39	2h	93	VAL	3.6
40	2i	40	LEU	3.6
44	1m	98	VAL	3.6
47	1p	17	TYR	3.6
50	2s	68	GLY	3.6
33	2b	111	ARG	3.6
54	2w	2	C	3.6
35	2d	48	ALA	3.6
45	2n	22	THR	3.6
51	1t	14	LYS	3.6
8	2I	12	LEU	3.6
35	1d	194	LEU	3.6
32	2a	1224	G	3.6
35	2d	168	ARG	3.6
57	1y	66	U	3.6
36	2e	20	GLN	3.6
40	2i	70	LYS	3.6
1	1A	1080	C	3.5
32	2a	1037	C	3.5
54	1w	4	C	3.5
1	1A	1073	A	3.5
7	2H	47	GLU	3.5
33	2b	170	GLU	3.5
7	2H	5	GLY	3.5
27	25	58	LEU	3.5
31	29	13	LYS	3.5
33	1b	165	VAL	3.5
34	2c	33	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
42	1k	14	VAL	3.5
52	1u	21	TYR	3.5
7	2H	145	ALA	3.5
32	2a	1452	C	3.5
2	2B	90	A	3.5
32	1a	1447	A	3.5
41	2j	68	HIS	3.5
17	2V	5	VAL	3.5
22	20	62	LEU	3.5
31	29	16	VAL	3.5
40	2i	86	VAL	3.5
51	2t	62	LEU	3.5
57	2y	69	G	3.5
1	1A	1077	A	3.5
32	1a	344	A	3.5
32	2a	1447	A	3.5
38	2g	34	GLY	3.5
36	1e	136	MET	3.5
31	29	14	CYS	3.5
38	2g	101	LEU	3.5
51	2t	68	LYS	3.5
19	2X	69	TYR	3.5
1	1A	1055	G	3.5
32	2a	980	C	3.5
33	2b	122	PHE	3.5
41	1j	47	PHE	3.5
38	2g	6	ARG	3.5
43	1l	10	LEU	3.5
43	1l	52	LEU	3.5
51	1t	71	THR	3.5
34	2c	41	GLY	3.5
42	2k	90	GLY	3.5
35	1d	110	PHE	3.5
45	1n	33	VAL	3.5
19	2X	91	ALA	3.5
34	1c	41	GLY	3.5
22	20	26	TYR	3.5
38	2g	44	TYR	3.5
32	2a	1149	C	3.5
45	2n	23	ARG	3.5
45	2n	45	ARG	3.5
51	1t	79	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
32	2a	1324	A	3.4
33	2b	201	ILE	3.4
43	2l	60	LEU	3.4
34	2c	195	VAL	3.4
40	1i	100	GLY	3.4
42	1k	15	ALA	3.4
44	1m	2	ALA	3.4
21	2Z	8	TYR	3.4
1	1A	1066	U	3.4
32	2a	1006	C	3.4
32	1a	102	G	3.4
32	1a	998	G	3.4
6	1G	80	PHE	3.4
4	2E	195	LEU	3.4
21	2Z	157	LEU	3.4
32	1a	1044	A	3.4
32	2a	1001	A	3.4
39	2h	112	LEU	3.4
21	2Z	96	VAL	3.4
21	2Z	126	VAL	3.4
34	1c	130	VAL	3.4
51	1t	80	ARG	3.4
32	1a	79	G	3.4
1	1A	2102	U	3.4
22	20	63	VAL	3.4
34	1c	153	VAL	3.4
7	2H	74	ASN	3.4
1	1A	2183	C	3.4
7	2H	171	LEU	3.4
11	2P	85	LEU	3.4
11	2P	138	LEU	3.4
19	2X	95	LEU	3.4
34	1c	128	PHE	3.4
34	2c	196	LEU	3.4
36	2e	123	LEU	3.4
48	1q	98	LEU	3.4
36	2e	55	VAL	3.4
45	2n	18	VAL	3.4
51	1t	17	ARG	3.4
20	2Y	55	TYR	3.4
1	1A	1082	U	3.4
1	1A	2137	C	3.4

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Mol	Chain	Res	Type	RSRZ
1	2A	2185	C	3.4
22	20	52	GLY	3.4
32	2a	1249	C	3.4
34	1c	81	GLY	3.4
40	2i	73	GLN	3.4
43	1l	64	TYR	3.4
44	2m	122	LYS	3.4
46	2o	55	GLY	3.4
14	2S	31	SER	3.4
3	2D	135	PHE	3.4
41	2j	32	ALA	3.4
44	2m	70	LEU	3.4
45	2n	10	ALA	3.4
1	1A	2153	G	3.4
1	2A	2153	G	3.4
32	1a	1285	A	3.4
34	1c	198	VAL	3.4
41	1j	34	VAL	3.4
1	1A	1065	U	3.4
1	2A	2130	U	3.4
7	2H	135	GLY	3.4
1	2A	645	C	3.4
39	2h	65	TYR	3.4
55	1x	67	C	3.4
45	1n	13	THR	3.4
42	1k	89	ALA	3.4
21	1Z	165	VAL	3.3
32	1a	138	G	3.4
1	2A	6	A	3.3
1	2A	901	A	3.3
32	1a	161	A	3.3
32	2a	1005	A	3.3
47	1p	59	TRP	3.3
6	1G	48	GLU	3.3
40	1i	49	PRO	3.3
40	2i	103	THR	3.3
52	2u	18	TYR	3.3
57	1y	41	C	3.3
41	2j	20	ALA	3.3
40	2i	33	PHE	3.3
1	1A	882	G	3.3
15	1T	70	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
33	2b	220	ASP	3.3
32	2a	1323	G	3.3
45	1n	56	VAL	3.3
54	2w	5	G	3.3
1	1A	1054	A	3.3
1	1A	2173	A	3.3
7	2H	126	PRO	3.3
32	2a	1248	A	3.3
34	2c	154	SER	3.3
1	1A	652(S)	C	3.3
9	2N	116	LEU	3.3
39	2h	6	ILE	3.3
44	1m	25	ILE	3.3
40	2i	80	GLY	3.3
33	2b	219	VAL	3.3
40	1i	113	LYS	3.3
43	1l	96	VAL	3.3
47	2p	20	VAL	3.3
1	1A	2152	G	3.3
1	2A	1117	G	3.3
21	2Z	4	ARG	3.3
32	1a	104	G	3.3
44	2m	104	ARG	3.3
51	2t	86	ARG	3.3
1	2A	895	U	3.3
11	2P	110	TYR	3.3
32	1a	163	C	3.3
50	2s	52	TYR	3.3
7	2H	33	LEU	3.3
34	1c	52	LEU	3.3
40	2i	56	LEU	3.3
26	24	48	ARG	3.3
40	2i	18	PHE	3.3
34	2c	105	GLU	3.3
1	2A	2131	G	3.3
32	2a	1142	G	3.3
26	14	52	THR	3.3
51	2t	77	ALA	3.3
34	2c	48	TYR	3.3
40	1i	114	TYR	3.3
40	2i	88	TYR	3.3
44	1m	96	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
12	2Q	65	PHE	3.3
40	2i	124	GLN	3.3
41	2j	23	ILE	3.3
42	2k	125	PHE	3.3
32	1a	1000	U	3.3
48	1q	35	VAL	3.3
1	1A	2186	G	3.3
32	2a	1061	G	3.3
35	2d	164	ALA	3.3
43	2l	56	ALA	3.3
44	2m	72	ALA	3.3
21	2Z	121	HIS	3.3
57	1y	43	C	3.3
9	2N	26	LEU	3.3
50	1s	22	LEU	3.3
33	2b	41	ILE	3.3
40	2i	75	ASP	3.3
7	1H	113	VAL	3.3
38	1g	4	ARG	3.3
1	2A	879	G	3.2
21	2Z	143	GLY	3.2
33	2b	207	ALA	3.2
7	2H	39	PRO	3.2
32	1a	150	C	3.2
7	2H	71	LEU	3.2
40	1i	79	LEU	3.2
29	27	47	ARG	3.2
9	2N	9	VAL	3.2
34	1c	194	GLY	3.2
40	2i	76	ALA	3.2
1	1A	1062	G	3.2
32	2a	79	G	3.2
36	1e	128	PRO	3.2
45	2n	54	PRO	3.2
34	1c	94	LEU	3.2
44	2m	93	ARG	3.2
52	1u	24	ARG	3.2
6	2G	39	ILE	3.2
8	2I	29	TYR	3.2
48	1q	90	ILE	3.2
45	2n	15	LYS	3.2
51	1t	74	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
52	2u	16	GLY	3.2
52	2u	17	THR	3.2
41	2j	69	ASN	3.2
36	2e	21	ALA	3.2
50	2s	13	ASP	3.2
1	1A	1056	G	3.2
1	1A	898	C	3.2
34	1c	34	LEU	3.2
34	2c	43	LEU	3.2
46	2o	31	LEU	3.2
33	2b	80	ILE	3.2
33	2b	92	TYR	3.2
34	2c	57	ILE	3.2
47	1p	48	TRP	3.2
57	1y	12	U	3.2
12	2Q	50	ALA	3.2
38	2g	2	ALA	3.2
40	1i	15	ALA	3.2
50	1s	4	SER	3.2
7	2H	30	LYS	3.2
46	2o	58	MET	3.2
1	1A	1176	G	3.2
2	2B	88	C	3.2
7	2H	89	ILE	3.2
7	2H	91	GLY	3.2
35	1d	5	ILE	3.2
40	1i	80	GLY	3.2
8	2I	96	ASP	3.2
14	2S	12	PHE	3.2
12	2Q	63	LYS	3.2
12	2Q	53	ALA	3.2
11	1P	105	LEU	3.2
32	1a	101	A	3.2
54	1w	31	A	3.2
35	1d	69	GLY	3.2
21	2Z	49	ARG	3.2
26	24	68	ARG	3.2
32	2a	1370	G	3.2
39	2h	37	ARG	3.2
45	2n	7	ILE	3.2
7	2H	65	HIS	3.2
33	2b	139	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
7	2H	49	VAL	3.2
21	1Z	39	VAL	3.2
7	2H	2	SER	3.2
5	2F	115	ALA	3.2
1	2A	1113	U	3.2
21	2Z	80	ARG	3.2
38	1g	84	ASN	3.2
1	2A	2801(A)	A	3.2
53	2v	15	A	3.2
7	2H	111	HIS	3.1
34	1c	14	ILE	3.1
38	1g	27	ILE	3.1
40	1i	33	PHE	3.1
52	2u	5	ASP	3.1
11	2P	105	LEU	3.1
33	2b	135	GLN	3.1
32	1a	174	C	3.1
7	2H	4	ILE	3.1
20	2Y	42	VAL	3.1
46	2o	60	VAL	3.1
38	2g	11	GLN	3.1
51	1t	20	LEU	3.1
54	2w	47	U	3.1
57	1y	45	U	3.1
34	2c	190	ARG	3.1
7	2H	10	PRO	3.1
11	2P	130	PHE	3.1
25	23	16	PRO	3.1
34	1c	174	PRO	3.1
32	2a	1022	G	3.1
32	2a	1068	G	3.1
34	2c	184	TYR	3.1
39	2h	28	ALA	3.1
40	2i	122	ALA	3.1
43	2l	43	VAL	3.1
44	1m	72	ALA	3.1
48	1q	77	VAL	3.1
49	1r	24	ALA	3.1
11	2P	93	GLY	3.1
12	2Q	61	GLY	3.1
7	2H	61	HIS	3.1
6	1G	139	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
23	11	98	LEU	3.1
7	2H	46	GLU	3.1
31	29	19	ARG	3.1
40	1i	47	LEU	3.1
41	2j	66	ARG	3.1
7	2H	70	THR	3.1
1	2A	2803	C	3.1
20	2Y	38	ILE	3.1
32	1a	1287	A	3.1
34	2c	182	ILE	3.1
53	1v	15	A	3.1
57	1y	76	A	3.1
7	2H	93	GLY	3.1
1	1A	2156	G	3.1
1	2A	2793	G	3.1
12	2Q	106	VAL	3.1
21	2Z	161	VAL	3.1
49	2r	57	GLY	3.1
32	1a	198	G	3.1
34	2c	201	TYR	3.1
32	1a	1040	U	3.1
51	2t	29	LYS	3.1
57	2y	60	U	3.1
40	1i	58	HIS	3.1
31	29	9	ARG	3.1
34	1c	190	ARG	3.1
41	2j	16	LEU	3.1
50	1s	12	ASP	3.1
50	1s	38	SER	3.1
36	2e	73	ASN	3.1
1	2A	1116	C	3.1
41	1j	96	ILE	3.1
41	2j	91	PRO	3.1
45	1n	7	ILE	3.1
1	2A	2750	A	3.1
8	2I	13	GLY	3.1
32	2a	1251	A	3.1
54	1w	20	U	3.1
7	2H	79	VAL	3.1
1	2A	2318	G	3.1
15	1T	108	ARG	3.1
35	2d	68	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
32	1a	216	G	3.1
32	2a	485	G	3.1
32	2a	1220	G	3.1
8	2I	35	LEU	3.1
35	1d	108	LEU	3.1
39	1h	112	LEU	3.1
45	2n	6	LEU	3.1
47	1p	22	THR	3.1
7	2H	97	ARG	3.1
34	1c	92	ALA	3.1
57	2y	9	A	3.1
23	2l	38	SER	3.0
8	2I	93	THR	3.0
21	1Z	150	LEU	3.0
33	2b	121	LEU	3.0
39	1h	133	LEU	3.0
47	1p	49	LEU	3.0
6	2G	24	GLY	3.0
41	2j	39	PRO	3.0
7	2H	69	ARG	3.0
52	1u	15	ARG	3.0
4	1E	77	ILE	3.0
23	2l	67	ILE	3.0
36	2e	76	ILE	3.0
1	2A	900	A	3.0
43	1l	43	VAL	3.0
7	2H	83	TYR	3.0
21	2Z	3	TYR	3.0
21	2Z	38	TYR	3.0
26	14	63	TYR	3.0
20	2Y	32	PRO	3.0
34	2c	205	GLY	3.0
40	2i	20	ARG	3.0
1	2A	2150	U	3.0
7	2H	144	VAL	3.0
7	2H	169	VAL	3.0
21	2Z	99	TYR	3.0
6	2G	17	PRO	3.0
41	2j	67	THR	3.0
1	2A	882	G	3.0
8	1I	30	LEU	3.0
21	1Z	51	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
36	2e	80	ILE	3.0
1	2A	1043	C	3.0
1	2A	2102	U	3.0
14	2S	3	ARG	3.0
25	23	29	ARG	3.0
33	2b	70	PHE	3.0
36	2e	84	PHE	3.0
41	1j	11	PHE	3.0
51	1t	86	ARG	3.0
35	1d	203	VAL	3.0
42	2k	114	VAL	3.0
50	1s	58	VAL	3.0
26	24	39	CYS	3.0
21	1Z	167	PRO	3.0
38	2g	85	TYR	3.0
40	2i	105	ASP	3.0
40	2i	123	PRO	3.0
1	1A	2207	G	3.0
1	2A	1112	G	3.0
54	2w	29	G	3.0
33	2b	185	ILE	3.0
32	1a	219	C	3.0
33	1b	59	GLU	3.0
45	1n	16	PHE	3.0
8	2I	3	VAL	3.0
47	1p	53	VAL	3.0
1	1A	1067	A	3.0
16	2U	2	PRO	3.0
36	1e	135	THR	3.0
44	2m	105	THR	3.0
40	1i	125	TYR	3.0
7	2H	7	LEU	3.0
21	2Z	125	LEU	3.0
5	1F	17	ARG	3.0
35	2d	122	ARG	3.0
52	1u	10	ARG	3.0
33	2b	116	GLU	3.0
35	1d	111	ALA	3.0
36	2e	17	ALA	3.0
48	2q	12	SER	3.0
38	1g	120	ILE	3.0
40	2i	77	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
41	1j	50	ILE	3.0
21	2Z	140	ASP	3.0
32	2a	1019	C	3.0
40	1i	57	GLY	3.0
44	2m	119	GLY	3.0
6	2G	160	VAL	3.0
34	2c	73	PRO	3.0
36	1e	51	VAL	3.0
34	2c	181	ASN	3.0
44	1m	109	THR	3.0
52	2u	8	THR	3.0
34	2c	126	ARG	3.0
35	2d	141	ARG	3.0
20	1Y	1	MET	2.9
21	2Z	67	LEU	2.9
34	1c	23	TYR	2.9
39	2h	2	LEU	2.9
34	2c	189	ALA	2.9
38	2g	117	ALA	2.9
1	1A	1091	G	2.9
1	1A	2124	G	2.9
1	1A	2155	G	2.9
2	2B	89	G	2.9
7	2H	48	GLY	2.9
15	2T	48	ILE	2.9
32	1a	70	G	2.9
40	2i	8	GLY	2.9
32	1a	201	C	2.9
1	1A	1078	U	2.9
38	2g	41	ARG	2.9
39	2h	116	LYS	2.9
16	2U	8	VAL	2.9
52	2u	9	ARG	2.9
36	1e	16	THR	2.9
48	1q	7	THR	2.9
1	2A	890	A	2.9
32	2a	1374	A	2.9
29	27	1	MET	2.9
35	1d	21	LEU	2.9
44	2m	96	LEU	2.9
50	2s	12	ASP	2.9
7	2H	104	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
7	2H	152	ARG	2.9
40	2i	128	ARG	2.9
8	2I	74	ASN	2.9
11	2P	96	THR	2.9
33	2b	113	HIS	2.9
41	2j	56	HIS	2.9
48	2q	11	VAL	2.9
21	2Z	160	GLY	2.9
52	1u	6	ARG	2.9
32	1a	93	G	2.9
32	2a	1154	G	2.9
6	2G	117	PHE	2.9
32	1a	100	C	2.9
32	1a	1158	C	2.9
32	1a	1452	C	2.9
8	1I	19	VAL	2.9
1	1A	1098	A	2.9
6	2G	43	LEU	2.9
36	1e	46	GLY	2.9
39	2h	133	LEU	2.9
40	1i	50	LEU	2.9
40	1i	85	LEU	2.9
21	2Z	9	TYR	2.9
47	1p	24	ALA	2.9
34	1c	8	ILE	2.9
31	29	20	HIS	2.9
41	2j	13	HIS	2.9
1	2A	652(V)	C	2.9
12	2Q	104	PHE	2.9
32	1a	78	G	2.9
32	2a	1009	G	2.9
32	2a	1283	G	2.9
7	2H	11	VAL	2.9
26	14	50	VAL	2.9
38	1g	6	ARG	2.9
53	2v	20	U	2.9
6	2G	73	ALA	2.9
40	2i	13	ALA	2.9
35	2d	38	TYR	2.9
40	2i	78	LYS	2.9
21	2Z	62	PRO	2.9
34	2c	83	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
32	2a	1284	C	2.9
32	2a	1326	C	2.9
1	2A	11	G	2.9
40	2i	37	PHE	2.9
12	1Q	15	GLY	2.9
33	1b	230	VAL	2.9
45	2n	51	GLY	2.9
45	2n	56	VAL	2.9
6	2G	3	LEU	2.9
8	2I	121	LYS	2.9
29	17	48	LYS	2.9
36	2e	12	LEU	2.9
39	2h	9	MET	2.9
48	2q	74	LEU	2.9
51	1t	16	HIS	2.9
33	1b	211	ILE	2.8
38	2g	30	ILE	2.8
7	2H	63	SER	2.8
7	2H	28	GLY	2.8
7	2H	166	GLY	2.8
11	2P	28	GLY	2.8
7	2H	27	LYS	2.8
7	2H	85	LYS	2.8
3	2D	185	VAL	2.8
21	2Z	94	GLU	2.8
32	1a	63	C	2.8
32	1a	1006	C	2.8
36	2e	28	PHE	2.8
55	2x	1	C	2.8
32	1a	927	G	2.8
32	1a	1385	G	2.8
8	2I	140	LEU	2.8
11	2P	140	ALA	2.8
12	2Q	136	ALA	2.8
20	1Y	67	LEU	2.8
40	2i	61	ALA	2.8
50	2s	75	ALA	2.8
51	1t	32	ALA	2.8
51	2t	24	LEU	2.8
1	1A	278	A	2.8
11	2P	137	LYS	2.8
39	1h	100	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
39	2h	35	ILE	2.8
40	1i	112	LYS	2.8
36	2e	114	GLY	2.8
40	2i	101	PHE	2.8
54	1w	2	C	2.8
16	2U	63	VAL	2.8
43	1l	24	VAL	2.8
45	1n	12	ARG	2.8
1	2A	1115	G	2.8
32	2a	1156	G	2.8
1	1A	1026	U	2.8
1	1A	1081	U	2.8
5	2F	162	LEU	2.8
9	1N	138	LEU	2.8
19	2X	66	LEU	2.8
23	2l	85	LEU	2.8
51	2t	44	ALA	2.8
31	29	11	CYS	2.8
1	1A	2176	A	2.8
32	2a	1016	A	2.8
4	1E	12	THR	2.8
42	1k	76	GLY	2.8
46	2o	89	GLY	2.8
34	1c	39	ILE	2.8
39	2h	38	ILE	2.8
21	2Z	122	ARG	2.8
1	1A	2150	U	2.8
32	2a	4	U	2.8
32	2a	1114	C	2.8
45	2n	16	PHE	2.8
38	2g	118	VAL	2.8
48	2q	77	VAL	2.8
12	2Q	107	ALA	2.8
41	2j	62	HIS	2.8
1	2A	274	G	2.8
6	2G	62	LEU	2.8
19	1X	95	LEU	2.8
34	2c	47	LEU	2.8
14	2S	22	GLY	2.8
34	1c	80	GLY	2.8
36	1e	97	GLY	2.8
1	1A	1088	A	2.8

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Mol	Chain	Res	Type	RSRZ
12	2Q	129	THR	2.8
4	2E	176	ILE	2.8
21	2Z	20	ARG	2.8
32	1a	160	A	2.8
35	2d	47	ARG	2.8
57	2y	7	A	2.8
43	2l	46	LYS	2.8
1	2A	277	C	2.8
26	14	59	PHE	2.8
21	2Z	47	VAL	2.8
27	15	60	VAL	2.8
42	1k	84	VAL	2.8
54	2w	56	C	2.8
55	1x	68	C	2.8
8	2I	38	LEU	2.8
41	1j	41	PRO	2.8
44	1m	90	LEU	2.8
46	1o	57	LEU	2.8
50	1s	30	LEU	2.8
32	1a	1274	G	2.8
48	1q	33	GLY	2.8
52	1u	4	GLY	2.8
7	2H	59	ARG	2.8
6	2G	63	ILE	2.8
6	2G	41	GLN	2.8
50	2s	69	HIS	2.8
7	2H	55	PRO	2.8
8	2I	127	VAL	2.8
35	2d	8	VAL	2.8
36	1e	96	PRO	2.8
50	2s	76	PRO	2.8
40	2i	111	ARG	2.8
41	2j	89	ASP	2.8
49	1r	85	LEU	2.8
50	2s	35	SER	2.8
52	2u	24	ARG	2.8
1	1A	1071	G	2.8
1	1A	1097	U	2.8
54	1w	15	G	2.8
35	2d	160	GLN	2.8
31	29	17	ILE	2.8
51	2t	63	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
50	2s	81	ARG	2.8
25	23	56	VAL	2.7
48	2q	56	VAL	2.7
35	2d	11	LEU	2.7
54	2w	45	U	2.7
44	2m	103	THR	2.7
9	2N	83	LYS	2.7
33	2b	211	ILE	2.7
39	1h	134	ILE	2.7
44	2m	92	HIS	2.7
50	2s	70	LYS	2.7
32	1a	197	A	2.7
32	1a	913	A	2.7
32	2a	1014	A	2.7
32	2a	1191	A	2.7
15	2T	71	GLY	2.7
26	14	64	GLY	2.7
30	28	28	GLY	2.7
46	1o	89	GLY	2.7
46	2o	2	PRO	2.7
34	1c	133	ALA	2.7
1	1A	1079	C	2.7
8	1I	136	VAL	2.7
21	1Z	141	VAL	2.7
22	20	60	PHE	2.7
35	1d	104	VAL	2.7
44	2m	101	GLN	2.7
21	1Z	1	MET	2.7
21	2Z	98	MET	2.7
34	2c	45	LYS	2.7
36	2e	50	GLU	2.7
45	2n	46	GLU	2.7
41	1j	46	ARG	2.7
51	2t	57	ARG	2.7
4	2E	134	ILE	2.7
11	2P	114	ILE	2.7
32	1a	64	G	2.7
32	1a	933	G	2.7
41	2j	6	ILE	2.7
50	1s	40	ILE	2.7
22	20	65	GLY	2.7
32	1a	228	A	2.7

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Mol	Chain	Res	Type	RSRZ
52	2u	11	GLY	2.7
7	2H	75	ALA	2.7
38	1g	152	ALA	2.7
41	2j	21	GLN	2.7
36	1e	84	PHE	2.7
38	1g	17	VAL	2.7
45	1n	4	LYS	2.7
11	2P	115	LEU	2.7
17	2V	71	LEU	2.7
25	23	23	LEU	2.7
34	2c	91	LEU	2.7
43	2l	52	LEU	2.7
11	2P	79	ARG	2.7
11	2P	102	ARG	2.7
52	2u	10	ARG	2.7
50	2s	14	HIS	2.7
4	2E	77	ILE	2.7
21	2Z	124	ILE	2.7
36	2e	129	ILE	2.7
40	1i	6	GLY	2.7
18	2W	80	PRO	2.7
43	1l	22	SER	2.7
48	2q	28	PRO	2.7
7	2H	32	GLU	2.7
43	1l	23	LYS	2.7
1	2A	1472	A	2.7
3	2D	130	ALA	2.7
12	2Q	93	TYR	2.7
32	2a	968	A	2.7
32	2a	969	A	2.7
33	2b	173	ALA	2.7
35	1d	38	TYR	2.7
46	2o	69	TYR	2.7
47	1p	38	TYR	2.7
48	1q	95	TYR	2.7
51	1t	76	ALA	2.7
6	2G	37	VAL	2.7
7	2H	125	VAL	2.7
33	1b	136	VAL	2.7
33	2b	105	PHE	2.7
45	2n	31	ARG	2.7
8	2I	75	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
15	1T	114	LEU	2.7
32	1a	194	C	2.7
50	2s	51	VAL	2.7
35	2d	120	LEU	2.7
49	2r	47	THR	2.7
1	1A	2172	U	2.7
7	2H	120	GLY	2.7
11	2P	24	GLY	2.7
51	2t	38	LYS	2.7
7	1H	4	ILE	2.7
33	1b	233	SER	2.7
33	2b	131	PRO	2.7
34	2c	174	PRO	2.7
51	2t	55	ILE	2.7
1	2A	880	G	2.7
14	2S	55	ALA	2.7
32	1a	230	G	2.7
44	1m	28	ALA	2.7
14	2S	92	TYR	2.7
32	1a	134	A	2.7
32	2a	1004	A	2.7
41	2j	12	ASP	2.7
7	2H	88	LEU	2.7
12	2Q	2	LEU	2.7
12	2Q	94	VAL	2.7
36	1e	69	VAL	2.7
38	1g	43	PHE	2.7
21	2Z	91	LEU	2.7
33	2b	47	THR	2.7
39	2h	119	LEU	2.7
41	1j	90	LEU	2.7
34	1c	89	GLU	2.7
12	2Q	33	GLY	2.7
52	1u	16	GLY	2.7
48	1q	2	PRO	2.7
7	2H	136	ILE	2.7
30	28	16	ILE	2.7
35	2d	70	ILE	2.7
51	1t	63	ILE	2.7
9	1N	102	ALA	2.7
14	2S	6	ALA	2.7
19	1X	46	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
35	2d	147	ALA	2.7
28	26	20	ASN	2.7
1	1A	1074	G	2.7
1	2A	1030	G	2.7
32	1a	625	G	2.7
32	2a	929	G	2.7
57	2y	59	U	2.7
1	1A	2790	A	2.7
1	2A	2298	A	2.7
19	1X	5	TYR	2.7
33	1b	135	GLN	2.7
35	1d	106	TYR	2.7
57	1y	9	A	2.7
3	2D	173	VAL	2.7
5	2F	114	VAL	2.7
36	2e	151	LEU	2.7
39	1h	26	VAL	2.7
41	1j	94	VAL	2.7
46	2o	85	LEU	2.7
32	1a	1008	C	2.7
35	2d	183	GLY	2.7
30	18	34	TRP	2.6
40	1i	10	ARG	2.6
44	2m	102	ARG	2.6
48	1q	30	PRO	2.6
7	2H	159	GLU	2.6
26	14	57	GLU	2.6
32	2a	1358	U	2.6
33	2b	223	ILE	2.6
44	1m	4	ILE	2.6
8	2I	83	ALA	2.6
9	1N	132	ALA	2.6
16	2U	42	ALA	2.6
42	2k	74	ALA	2.6
41	1j	62	HIS	2.6
32	2a	1221	G	2.6
54	1w	1	G	2.6
54	2w	69	G	2.6
1	2A	899	A	2.6
12	2Q	17	LEU	2.6
12	2Q	59	ARG	2.6
18	1W	71	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
32	1a	149	A	2.6
36	1e	59	GLY	2.6
38	2g	12	LEU	2.6
40	2i	99	LEU	2.6
44	1m	26	GLY	2.6
45	1n	47	LEU	2.6
48	1q	89	LEU	2.6
48	2q	91	ARG	2.6
50	2s	5	LEU	2.6
51	2t	99	LEU	2.6
1	2A	893	C	2.6
32	2a	999	C	2.6
35	1d	181	MET	2.6
21	1Z	149	SER	2.6
43	2l	13	LYS	2.6
44	1m	122	LYS	2.6
1	1A	1963	U	2.6
28	26	42	TRP	2.6
50	2s	34	TRP	2.6
10	2O	30	ALA	2.6
23	2l	13	ILE	2.6
34	1c	100	ALA	2.6
35	1d	2	GLY	2.6
42	1k	87	THR	2.6
11	2P	147	LEU	2.6
1	2A	1032	A	2.6
3	2D	79	VAL	2.6
8	2I	92	VAL	2.6
33	2b	133	LYS	2.6
35	2d	78	LEU	2.6
46	2o	66	LEU	2.6
55	2x	46	G	2.6
4	2E	32	PRO	2.6
8	1I	74	ASN	2.6
43	2l	48	PRO	2.6
8	1I	26	ALA	2.6
15	2T	111	ARG	2.6
23	1l	24	ALA	2.6
38	2g	155	ARG	2.6
49	1r	73	ALA	2.6
21	2Z	2	GLU	2.6
40	1i	24	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
52	2u	12	LYS	2.6
5	2F	41	LEU	2.6
7	2H	94	TYR	2.6
7	2H	123	PHE	2.6
9	2N	8	GLN	2.6
16	2U	20	LEU	2.6
22	20	59	LEU	2.6
23	11	94	LEU	2.6
33	2b	154	LEU	2.6
34	1c	32	LEU	2.6
34	1c	87	LEU	2.6
49	1r	31	LEU	2.6
1	1A	899	A	2.6
1	1A	2833	G	2.6
1	1A	1100	C	2.6
21	2Z	167	PRO	2.6
32	1a	1007	C	2.6
32	2a	994	A	2.6
32	2a	1349	A	2.6
47	1p	41	PRO	2.6
53	1v	24	A	2.6
54	1w	3	C	2.6
54	1w	73	A	2.6
11	2P	94	GLU	2.6
19	2X	68	ARG	2.6
29	27	45	ALA	2.6
6	1G	77	ILE	2.6
6	2G	157	ILE	2.6
3	2D	110	GLY	2.6
19	1X	94	GLY	2.6
34	2c	96	GLY	2.6
35	2d	134	ASP	2.6
31	29	29	ASN	2.6
33	2b	25	ASN	2.6
35	2d	154	ASN	2.6
41	1j	30	SER	2.6
4	1E	183	LEU	2.6
4	2E	53	PRO	2.6
8	2I	30	LEU	2.6
30	28	61	LEU	2.6
33	2b	91	PRO	2.6
46	2o	57	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
21	2Z	128	VAL	2.6
26	24	56	VAL	2.6
33	2b	136	VAL	2.6
34	2c	75	VAL	2.6
38	1g	69	VAL	2.6
39	2h	19	VAL	2.6
7	2H	77	LYS	2.6
25	23	30	ARG	2.6
32	1a	220	G	2.6
32	1a	1353	G	2.6
32	2a	102	G	2.6
32	2a	553	A	2.6
32	2a	1011	G	2.6
32	2a	1179	A	2.6
32	2a	1288	A	2.6
32	2a	1363	C	2.6
44	2m	121	LYS	2.6
22	20	61	ALA	2.6
33	1b	123	ALA	2.6
34	2c	194	GLY	2.6
33	2b	124	SER	2.6
34	2c	20	SER	2.6
50	2s	48	THR	2.6
35	1d	150	GLU	2.6
33	2b	144	ARG	2.6
40	2i	127	LYS	2.6
46	1o	88	ARG	2.6
46	2o	68	ARG	2.6
33	2b	142	LEU	2.6
38	2g	58	PRO	2.6
12	2Q	103	MET	2.6
14	2S	14	VAL	2.6
35	2d	121	VAL	2.6
50	1s	10	PHE	2.6
36	1e	60	TYR	2.6
1	1A	2803	C	2.6
1	1A	1083	U	2.6
32	2a	1017	G	2.6
32	2a	1151	A	2.6
9	2N	69	GLN	2.6
11	1P	93	GLY	2.6
25	23	27	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
33	2b	95	GLN	2.6
33	2b	177	ALA	2.6
35	1d	143	GLY	2.6
36	2e	85	GLY	2.6
45	1n	48	ALA	2.6
33	2b	231	GLU	2.6
24	12	41	ILE	2.6
35	2d	18	LYS	2.6
38	2g	42	ILE	2.6
39	2h	111	ILE	2.6
41	1j	57	LYS	2.6
9	1N	32	THR	2.5
5	2F	65	TRP	2.5
9	2N	112	LEU	2.5
38	1g	99	LEU	2.5
40	1i	99	LEU	2.5
40	2i	96	LEU	2.5
12	2Q	29	PHE	2.5
30	18	4	MET	2.5
30	28	25	MET	2.5
36	2e	136	MET	2.5
38	1g	21	VAL	2.5
38	1g	73	MET	2.5
38	2g	21	VAL	2.5
7	2H	127	GLU	2.5
32	1a	217	C	2.5
32	2a	995	C	2.5
34	2c	185	GLY	2.5
41	1j	93	GLY	2.5
41	2j	36	GLY	2.5
54	2w	67	C	2.5
1	2A	652(A)	A	2.5
32	2a	978	A	2.5
32	2a	1057	G	2.5
34	2c	63	ASN	2.5
40	2i	45	ALA	2.5
47	1p	7	ALA	2.5
50	2s	38	SER	2.5
52	1u	17	THR	2.5
35	1d	136	PRO	2.5
1	2A	271(K)	U	2.5
1	2A	2132	U	2.5

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Mol	Chain	Res	Type	RSRZ
16	1U	39	LEU	2.5
22	20	37	LEU	2.5
28	26	11	LEU	2.5
34	1c	175	LEU	2.5
36	2e	142	LEU	2.5
38	2g	22	LEU	2.5
45	1n	61	TRP	2.5
46	1o	32	LEU	2.5
33	2b	16	HIS	2.5
23	21	51	VAL	2.5
3	2D	189	CYS	2.5
7	2H	78	GLY	2.5
9	1N	14	VAL	2.5
39	2h	44	PHE	2.5
20	2Y	79	CYS	2.5
40	2i	69	GLY	2.5
48	1q	8	GLY	2.5
8	2I	82	ARG	2.5
17	2V	91	TYR	2.5
25	23	44	ARG	2.5
35	1d	68	TYR	2.5
38	2g	119	ARG	2.5
40	2i	89	ASN	2.5
1	2A	1445	A	2.5
32	2a	1180	A	2.5
36	2e	138	ALA	2.5
51	1t	78	ALA	2.5
32	1a	1392	G	2.5
54	2w	15	G	2.5
54	2w	30	G	2.5
7	2H	129	THR	2.5
22	20	43	THR	2.5
34	1c	124	ILE	2.5
1	1A	895	U	2.5
31	29	15	LYS	2.5
5	2F	24	LEU	2.5
7	1H	166	GLY	2.5
42	2k	76	GLY	2.5
46	1o	81	LEU	2.5
48	2q	75	ARG	2.5
3	2D	142	VAL	2.5
21	1Z	104	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
36	1e	82	VAL	2.5
1	1A	1053	C	2.5
3	2D	84	TYR	2.5
5	1F	13	SER	2.5
18	1W	28	SER	2.5
21	2Z	17	ALA	2.5
30	28	24	ALA	2.5
33	1b	31	TYR	2.5
38	2g	121	ALA	2.5
51	1t	70	SER	2.5
51	2t	52	ALA	2.5
1	2A	870	A	2.5
32	1a	1004	A	2.5
32	1a	1350	A	2.5
1	2A	2805	G	2.5
32	1a	61	G	2.5
32	2a	1368	G	2.5
32	2a	1371	G	2.5
33	1b	185	ILE	2.5
35	1d	40	PRO	2.5
43	2l	31	PRO	2.5
40	2i	120	ARG	2.5
51	1t	89	ARG	2.5
35	1d	180	GLY	2.5
38	1g	82	GLY	2.5
40	2i	39	GLY	2.5
24	22	60	LEU	2.5
3	2D	51	VAL	2.5
7	1H	76	VAL	2.5
7	2H	18	GLU	2.5
8	2I	117	GLU	2.5
8	2I	144	VAL	2.5
21	2Z	42	VAL	2.5
23	11	51	VAL	2.5
33	1b	15	VAL	2.5
39	2h	95	VAL	2.5
39	2h	138	TRP	2.5
40	2i	28	VAL	2.5
49	1r	86	VAL	2.5
50	2s	9	VAL	2.5
30	28	29	LYS	2.5
1	2A	857	C	2.5

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Mol	Chain	Res	Type	RSRZ
32	2a	175	C	2.5
12	2Q	110	THR	2.5
16	1U	69	CYS	2.5
22	10	43	THR	2.5
27	25	29	THR	2.5
38	2g	24	THR	2.5
7	2H	21	PRO	2.5
7	2H	95	ARG	2.5
8	1I	132	PRO	2.5
31	29	35	ARG	2.5
34	2c	21	ARG	2.5
36	2e	77	PRO	2.5
38	1g	32	ARG	2.5
38	1g	78	ARG	2.5
38	2g	120	ILE	2.5
41	2j	75	ILE	2.5
1	1A	2191	G	2.5
1	2A	875	G	2.5
1	2A	2792	G	2.5
13	2R	61	HIS	2.5
15	1T	38	ASN	2.5
32	2a	1133	G	2.5
40	2i	30	GLY	2.5
21	1Z	169	GLU	2.5
40	2i	35	GLU	2.5
13	2R	65	LEU	2.5
21	2Z	46	LYS	2.5
39	2h	36	LEU	2.5
51	1t	24	LEU	2.5
9	2N	90	MET	2.5
42	1k	73	MET	2.5
51	1t	85	MET	2.5
7	1H	2	SER	2.5
7	2H	50	VAL	2.5
21	2Z	44	PHE	2.5
31	29	3	VAL	2.5
39	2h	53	VAL	2.5
42	2k	43	SER	2.5
4	1E	46	ALA	2.5
5	1F	26	ALA	2.5
5	1F	111	ALA	2.5
20	2Y	48	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
34	2c	200	ALA	2.5
51	1t	67	ALA	2.5
1	2A	1119	C	2.5
35	1d	3	ARG	2.5
39	2h	122	ARG	2.5
11	2P	58	THR	2.5
36	2e	75	THR	2.5
45	2n	21	TYR	2.5
47	1p	69	THR	2.5
8	1I	109	ILE	2.5
10	1O	21	CYS	2.5
15	2T	110	ILE	2.5
30	28	20	GLY	2.5
33	2b	19	HIS	2.5
34	2c	6	HIS	2.5
39	1h	43	GLY	2.5
50	1s	69	HIS	2.5
48	2q	59	ILE	2.5
32	1a	145	G	2.5
32	1a	1009	G	2.5
32	1a	1323	G	2.5
32	2a	1108	G	2.5
32	2a	1353	G	2.5
1	2A	877	U	2.5
55	2x	47	U	2.5
4	2E	78	LEU	2.5
8	1I	35	LEU	2.5
8	2I	114	LEU	2.5
9	2N	91	LEU	2.5
35	1d	102	ASP	2.5
48	2q	76	LEU	2.5
3	2D	272	ALA	2.4
6	2G	163	ALA	2.4
9	2N	103	VAL	2.4
11	2P	125	VAL	2.4
35	1d	198	VAL	2.4
39	1h	31	PHE	2.4
48	2q	27	PHE	2.4
10	2O	108	GLU	2.4
35	2d	145	GLU	2.4
1	2A	1118	C	2.4
1	2A	2896	C	2.4

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Mol	Chain	Res	Type	RSRZ
9	2N	108	PRO	2.4
11	2P	30	THR	2.4
32	2a	1115	C	2.4
47	2p	59	TRP	2.4
17	2V	54	GLY	2.4
33	2b	89	GLY	2.4
36	2e	60	TYR	2.4
40	2i	117	HIS	2.4
44	1m	89	GLY	2.4
32	2a	1146	A	2.4
33	2b	42	ILE	2.4
43	2l	7	ILE	2.4
47	1p	76	GLN	2.4
1	1A	900	A	2.4
43	2l	37	CYS	2.4
32	1a	1529	G	2.4
34	2c	140	ARG	2.4
39	2h	127	LEU	2.4
9	1N	1	MET	2.4
18	1W	50	VAL	2.4
36	2e	67	VAL	2.4
38	2g	134	ALA	2.4
48	2q	35	VAL	2.4
11	2P	84	ASN	2.4
42	2k	117	ASN	2.4
23	2l	87	PRO	2.4
34	2c	13	GLY	2.4
43	1l	29	GLY	2.4
45	1n	28	GLY	2.4
32	2a	217	C	2.4
32	2a	1223	C	2.4
32	2a	1321	C	2.4
54	2w	13	C	2.4
11	1P	102	ARG	2.4
15	2T	115	ARG	2.4
16	2U	17	ILE	2.4
39	2h	86	ILE	2.4
41	2j	50	ILE	2.4
45	1n	42	ILE	2.4
51	2t	100	ILE	2.4
32	2a	977	A	2.4
31	29	33	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
35	1d	99	SER	2.4
21	1Z	24	LEU	2.4
32	1a	1530	G	2.4
35	1d	186	LEU	2.4
51	2t	9	ASN	2.4
23	2l	54	ALA	2.4
33	1b	105	PHE	2.4
34	2c	37	GLN	2.4
51	1t	12	ALA	2.4
51	2t	40	ALA	2.4
8	2l	19	VAL	2.4
12	2Q	102	VAL	2.4
28	26	48	VAL	2.4
34	2c	114	PRO	2.4
35	1d	7	PRO	2.4
36	1e	55	VAL	2.4
3	1D	50	THR	2.4
26	24	19	GLY	2.4
41	2j	92	THR	2.4
6	1G	116	ASP	2.4
1	1A	652(T)	C	2.4
32	1a	175	C	2.4
32	1a	177	C	2.4
32	1a	930	C	2.4
32	1a	1367	C	2.4
32	2a	1096	C	2.4
41	1j	70	ARG	2.4
33	2b	31	TYR	2.4
40	1i	5	TYR	2.4
48	1q	32	TYR	2.4
35	2d	126	ILE	2.4
1	2A	2753	A	2.4
2	2B	59	A	2.4
3	2D	37	LEU	2.4
13	2R	71	GLN	2.4
3	2D	247	ALA	2.4
4	1E	68	ALA	2.4
12	2Q	1	MET	2.4
7	2H	142	GLY	2.4
21	2Z	7	ALA	2.4
35	2d	33	MET	2.4
34	1c	78	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
38	1g	25	ALA	2.4
40	1i	72	GLY	2.4
46	2o	16	ALA	2.4
47	1p	64	ALA	2.4
50	1s	75	ALA	2.4
7	2H	114	VAL	2.4
9	2N	61	ARG	2.4
11	2P	71	VAL	2.4
12	2Q	69	PHE	2.4
14	2S	46	VAL	2.4
14	2S	69	VAL	2.4
20	2Y	30	VAL	2.4
33	2b	71	VAL	2.4
33	2b	153	ARG	2.4
40	1i	109	VAL	2.4
48	1q	11	VAL	2.4
50	2s	37	ARG	2.4
1	1A	894	C	2.4
1	1A	2794	C	2.4
32	1a	165	C	2.4
32	1a	178	C	2.4
32	1a	1038	C	2.4
32	1a	1039	C	2.4
32	1a	1259	C	2.4
32	2a	1354	C	2.4
15	1T	106	SER	2.4
8	2I	88	ILE	2.4
9	1N	13	TRP	2.4
12	2Q	66	ILE	2.4
35	1d	4	TYR	2.4
35	1d	20	TYR	2.4
41	1j	4	ILE	2.4
1	1A	878	A	2.4
32	1a	202	U	2.4
33	1b	134	GLU	2.4
8	1I	123	LEU	2.4
18	1W	36	LEU	2.4
19	1X	70	LEU	2.4
20	2Y	14	LEU	2.4
23	11	85	LEU	2.4
39	2h	39	LEU	2.4
42	2k	66	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
9	2N	84	LYS	2.4
14	2S	93	LYS	2.4
19	1X	4	ALA	2.4
26	24	55	ARG	2.4
36	1e	15	ARG	2.4
37	1f	92	LYS	2.4
51	2t	22	ARG	2.4
33	2b	101	MET	2.4
47	1p	15	PRO	2.4
1	2A	855	G	2.4
3	2D	18	VAL	2.4
18	1W	21	VAL	2.4
25	23	6	VAL	2.4
32	1a	105	G	2.4
32	1a	306	G	2.4
32	1a	1138	G	2.4
32	2a	1117	G	2.4
33	1b	219	VAL	2.4
40	1i	26	VAL	2.4
50	2s	45	VAL	2.4
1	2A	2794	C	2.4
15	2T	90	GLN	2.4
23	21	86	SER	2.4
32	1a	193	C	2.4
32	1a	1362	C	2.4
32	1a	1389	C	2.4
12	2Q	47	ILE	2.4
32	2a	981	U	2.4
36	2e	24	ARG	2.4
43	2l	95	GLY	2.4
1	2A	878	A	2.4
3	2D	77	ALA	2.4
38	2g	7	ALA	2.4
48	2q	47	PRO	2.4
8	2I	86	THR	2.4
25	13	40	THR	2.4
34	2c	15	THR	2.4
48	2q	7	THR	2.4
4	1E	47	VAL	2.4
9	2N	98	VAL	2.4
32	2a	1185	G	2.4
33	2b	146	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
39	2h	118	VAL	2.4
43	2l	32	PHE	2.4
45	2n	33	VAL	2.4
47	2p	2	VAL	2.4
32	1a	1042	G	2.4
50	1s	64	GLU	2.4
35	1d	154	ASN	2.4
26	14	68	ARG	2.3
32	1a	401	C	2.3
32	1a	1325	C	2.3
32	1a	1366	C	2.3
32	2a	1118	C	2.3
32	2a	1388	C	2.3
34	1c	179	ARG	2.3
34	2c	156	ARG	2.3
40	2i	51	ARG	2.3
15	2T	102	ILE	2.3
4	2E	148	GLY	2.3
12	1Q	93	TYR	2.3
11	2P	120	ALA	2.3
17	1V	20	LEU	2.3
25	23	12	PRO	2.3
33	2b	86	GLU	2.3
36	2e	54	ALA	2.3
40	2i	50	LEU	2.3
40	2i	110	GLU	2.3
41	2j	25	GLU	2.3
48	2q	6	LEU	2.3
51	2t	49	ALA	2.3
51	2t	67	ALA	2.3
1	1A	1847	A	2.3
32	1a	622	A	2.3
32	1a	1225	A	2.3
32	2a	1130	A	2.3
38	2g	56	GLN	2.3
41	2j	87	THR	2.3
3	2D	98	VAL	2.3
3	2D	138	VAL	2.3
5	2F	183	VAL	2.3
7	1H	169	VAL	2.3
10	1O	99	PHE	2.3
11	2P	126	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
21	1Z	52	SER	2.3
30	28	48	PHE	2.3
34	2c	144	SER	2.3
36	2e	45	PHE	2.3
36	2e	125	SER	2.3
38	2g	91	VAL	2.3
51	1t	75	ASN	2.3
32	1a	378	G	2.3
32	2a	77	G	2.3
32	2a	1058	G	2.3
32	2a	1184	G	2.3
11	1P	143	GLY	2.3
32	1a	1234	C	2.3
32	2a	422	C	2.3
34	2c	155	GLY	2.3
23	11	58	ILE	2.3
30	28	41	ILE	2.3
36	2e	131	ILE	2.3
41	1j	68	HIS	2.3
41	1j	98	ILE	2.3
11	1P	110	TYR	2.3
5	2F	170	LEU	2.3
8	2I	101	LEU	2.3
11	2P	76	LYS	2.3
11	2P	122	PRO	2.3
35	1d	207	TYR	2.3
40	1i	36	TYR	2.3
10	2O	76	ALA	2.3
14	2S	58	LEU	2.3
16	2U	41	ALA	2.3
33	1b	187	LEU	2.3
34	2c	61	ALA	2.3
35	2d	94	LEU	2.3
3	2D	70	TRP	2.3
5	2F	112	MET	2.3
32	2a	90	U	2.3
40	1i	27	THR	2.3
41	2j	15	THR	2.3
44	1m	103	THR	2.3
32	1a	152	A	2.3
32	2a	949	A	2.3
50	2s	66	MET	2.3

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Mol	Chain	Res	Type	RSRZ
5	2F	57	VAL	2.3
15	2T	70	VAL	2.3
34	1c	86	VAL	2.3
34	2c	173	VAL	2.3
38	1g	33	ASP	2.3
46	1o	60	VAL	2.3
34	1c	19	GLU	2.3
1	1A	2893	G	2.3
32	1a	68	G	2.3
50	2s	72	GLY	2.3
7	2H	62	LYS	2.3
51	1t	73	HIS	2.3
6	2G	133	LEU	2.3
8	2I	28	ASN	2.3
18	1W	19	LEU	2.3
21	2Z	163	LEU	2.3
23	21	64	ALA	2.3
25	23	15	TYR	2.3
30	18	64	TYR	2.3
31	29	24	TYR	2.3
32	2a	1219	U	2.3
33	2b	120	ALA	2.3
34	2c	59	ARG	2.3
35	2d	64	LEU	2.3
37	1f	21	LEU	2.3
37	2f	59	TYR	2.3
45	1n	57	ARG	2.3
45	2n	53	LEU	2.3
51	2t	12	ALA	2.3
41	2j	100	THR	2.3
34	2c	22	TRP	2.3
3	2D	229	VAL	2.3
4	1E	150	VAL	2.3
27	25	60	VAL	2.3
20	2Y	25	GLY	2.3
22	20	69	PHE	2.3
40	1i	37	PHE	2.3
48	2q	5	VAL	2.3
44	1m	38	GLY	2.3
1	1A	2792	G	2.3
32	1a	107	G	2.3
32	1a	1233	G	2.3

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Mol	Chain	Res	Type	RSRZ
32	2a	506	G	2.3
32	2a	998	G	2.3
54	1w	30	G	2.3
9	2N	85	ILE	2.3
18	2W	87	PRO	2.3
32	1a	1354	C	2.3
32	2a	1045	C	2.3
33	2b	36	ARG	2.3
36	2e	132	ALA	2.3
50	1s	50	ALA	2.3
7	2H	80	SER	2.3
11	2P	32	THR	2.3
12	2Q	79	LEU	2.3
17	2V	62	LEU	2.3
21	2Z	59	LEU	2.3
26	14	67	TYR	2.3
35	1d	101	LEU	2.3
40	1i	88	TYR	2.3
48	1q	84	LEU	2.3
48	2q	22	LEU	2.3
48	1q	97	SER	2.3
50	1s	48	THR	2.3
50	1s	52	TYR	2.3
51	1t	53	LEU	2.3
45	1n	17	LYS	2.3
32	2a	1357	A	2.3
33	2b	97	TRP	2.3
41	2j	93	GLY	2.3
50	2s	82	GLY	2.3
9	1N	117	PHE	2.3
12	1Q	58	PHE	2.3
21	1Z	88	PHE	2.3
23	21	70	VAL	2.3
33	2b	93	VAL	2.3
35	1d	140	VAL	2.3
23	21	50	ARG	2.3
41	2j	9	ARG	2.3
7	2H	117	PRO	2.3
1	2A	2870	C	2.3
26	14	65	ASP	2.3
29	27	44	PRO	2.3
33	2b	37	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
45	1n	14	PRO	2.3
21	2Z	133	ILE	2.3
32	1a	1342	C	2.3
32	1a	1456	G	2.3
32	2a	174	C	2.3
32	2a	933	G	2.3
32	2a	1160	G	2.3
54	2w	19	G	2.3
45	2n	50	LYS	2.3
9	2N	102	ALA	2.3
21	2Z	41	LEU	2.3
30	18	37	SER	2.3
36	1e	146	ALA	2.3
40	1i	82	ALA	2.3
40	1i	122	ALA	2.3
38	1g	12	LEU	2.3
40	1i	40	LEU	2.3
25	23	60	GLU	2.3
32	1a	1020	U	2.3
45	1n	23	ARG	2.3
4	1E	196	VAL	2.3
7	2H	133	VAL	2.3
11	1P	146	VAL	2.3
25	23	59	VAL	2.3
32	2a	1236	A	2.3
36	1e	6	PHE	2.3
40	1i	28	VAL	2.3
41	1j	49	VAL	2.3
43	1l	39	VAL	2.3
44	2m	74	VAL	2.3
48	2q	57	VAL	2.3
55	1x	38	A	2.3
40	1i	116	LYS	2.3
40	1i	123	PRO	2.3
32	1a	307	C	2.3
10	2O	51	ALA	2.3
12	2Q	64	ILE	2.3
32	2a	1153	C	2.3
13	1R	62	ALA	2.3
13	1R	101	ALA	2.3
22	20	2	ALA	2.3
34	2c	77	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
39	1h	38	ILE	2.3
40	2i	55	ALA	2.3
41	1j	32	ALA	2.3
42	2k	21	ILE	2.3
6	2G	152	LEU	2.2
8	2I	47	LEU	2.2
12	1Q	43	THR	2.2
32	1a	199	G	2.3
32	1a	226	G	2.3
34	2c	191	THR	2.2
35	2d	176	LEU	2.2
36	1e	53	LEU	2.2
38	2g	54	THR	2.2
55	1x	46	G	2.3
12	2Q	125	LEU	2.2
19	1X	66	LEU	2.2
7	2H	167	GLU	2.2
12	2Q	122	GLY	2.2
34	2c	171	GLY	2.2
35	2d	130	GLY	2.2
43	1l	103	GLY	2.2
44	2m	91	ARG	2.2
7	2H	164	TYR	2.2
29	17	1	MET	2.2
18	1W	111	HIS	2.2
33	1b	16	HIS	2.2
42	2k	119	CYS	2.2
46	1o	46	HIS	2.2
33	1b	133	LYS	2.2
45	2n	58	LYS	2.2
1	2A	1847	A	2.2
1	2A	2758	A	2.2
23	2l	60	PHE	2.2
32	1a	151	A	2.2
32	2a	1280	A	2.2
40	2i	26	VAL	2.2
40	2i	53	VAL	2.2
50	2s	58	VAL	2.2
54	1w	7	A	2.2
42	1k	78	GLN	2.2
33	1b	124	SER	2.2
3	1D	165	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
12	1Q	66	ILE	2.2
12	2Q	120	ILE	2.2
35	1d	163	GLU	2.2
20	1Y	65	ALA	2.2
1	2A	272(A)	U	2.2
6	2G	136	ARG	2.2
32	2a	1066	C	2.2
32	2a	1128	C	2.2
34	1c	126	ARG	2.2
35	1d	141	ARG	2.2
1	2A	1883	G	2.2
7	2H	13	LYS	2.2
13	1R	10	LEU	2.2
27	15	30	LEU	2.2
32	1a	928	G	2.2
32	2a	9	G	2.2
34	1c	178	LEU	2.2
36	1e	31	LEU	2.2
41	2j	71	LEU	2.2
46	2o	61	GLY	2.2
5	2F	99	TYR	2.2
9	1N	106	MET	2.2
18	1W	38	TYR	2.2
26	24	67	TYR	2.2
29	17	22	MET	2.2
40	1i	91	ASP	2.2
7	1H	144	VAL	2.2
8	2I	18	VAL	2.2
33	1b	7	VAL	2.2
33	1b	52	GLU	2.2
35	1d	105	VAL	2.2
6	2G	80	PHE	2.2
32	2a	983	A	2.2
11	2P	65	ARG	2.2
45	2n	32	SER	2.2
48	2q	39	SER	2.2
25	23	17	LYS	2.2
5	2F	51	THR	2.2
17	1V	4	ILE	2.2
17	1V	45	THR	2.2
21	2Z	152	ALA	2.2
37	2f	8	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
38	1g	24	THR	2.2
39	1h	7	ALA	2.2
40	1i	118	LYS	2.2
34	1c	159	GLY	2.2
32	2a	92	C	2.2
32	2a	979	C	2.2
32	2a	1217	C	2.2
47	2p	69	THR	2.2
51	1t	33	ILE	2.2
3	2D	177	LEU	2.2
3	2D	215	LEU	2.2
8	2I	128	LEU	2.2
36	2e	139	LEU	2.2
37	2f	30	LEU	2.2
47	1p	16	HIS	2.2
1	2A	1470	G	2.2
32	1a	146	G	2.2
32	1a	156	G	2.2
32	1a	166	G	2.2
32	2a	1197	G	2.2
7	2H	58	GLU	2.2
26	24	57	GLU	2.2
34	2c	162	GLN	2.2
30	28	64	TYR	2.2
47	2p	32	TYR	2.2
48	2q	95	TYR	2.2
11	1P	145	PRO	2.2
40	1i	21	PRO	2.2
51	2t	98	PRO	2.2
52	2u	15	ARG	2.2
4	2E	31	CYS	2.2
8	1I	15	VAL	2.2
11	2P	83	VAL	2.2
13	1R	97	VAL	2.2
14	2S	65	VAL	2.2
23	2I	49	VAL	2.2
31	19	7	VAL	2.2
34	1c	97	LYS	2.2
38	1g	141	VAL	2.2
51	1t	88	VAL	2.2
47	1p	61	SER	2.2
1	1A	1046	A	2.2

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Mol	Chain	Res	Type	RSRZ
1	2A	225	A	2.2
1	2A	528	A	2.2
32	1a	172	A	2.2
54	1w	23	A	2.2
6	2G	85	GLY	2.2
48	2q	54	GLY	2.2
6	1G	163	ALA	2.2
16	2U	21	ALA	2.2
3	2D	174	ILE	2.2
7	2H	122	THR	2.2
8	1I	146	ALA	2.2
28	26	47	THR	2.2
34	2c	60	ALA	2.2
34	2c	149	ALA	2.2
37	2f	29	ALA	2.2
41	2j	73	ASP	2.2
42	1k	74	ALA	2.2
43	1l	26	ALA	2.2
32	2a	1367	C	2.2
38	1g	153	HIS	2.2
47	1p	4	ILE	2.2
8	1I	5	LEU	2.2
16	2U	95	LEU	2.2
23	2I	73	LEU	2.2
35	1d	78	LEU	2.2
36	1e	20	GLN	2.2
51	2t	90	GLN	2.2
11	2P	60	MET	2.2
32	1a	922	G	2.2
38	2g	36	LYS	2.2
40	2i	93	ARG	2.2
48	1q	68	ARG	2.2
51	1t	81	LYS	2.2
54	2w	10	G	2.2
32	2a	1446	U	2.2
34	2c	23	TYR	2.2
42	1k	25	TYR	2.2
47	2p	58	TYR	2.2
3	1D	221	VAL	2.2
8	2I	21	VAL	2.2
8	2I	142	VAL	2.2
9	1N	55	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
15	2T	66	VAL	2.2
17	2V	61	VAL	2.2
19	1X	12	VAL	2.2
25	23	36	VAL	2.2
34	1c	68	VAL	2.2
34	2c	120	VAL	2.2
44	2m	98	VAL	2.2
24	12	37	PHE	2.2
27	25	54	GLY	2.2
33	2b	152	PHE	2.2
35	1d	41	GLY	2.2
36	1e	26	PHE	2.2
5	2F	177	ALA	2.2
21	1Z	151	HIS	2.2
26	24	27	THR	2.2
32	1a	262	A	2.2
32	1a	1005	A	2.2
32	1a	1261	A	2.2
32	2a	1229	A	2.2
42	1k	68	ALA	2.2
42	2k	68	ALA	2.2
45	2n	49	HIS	2.2
46	1o	16	ALA	2.2
7	2H	162	ILE	2.2
9	1N	71	ILE	2.2
24	22	50	ILE	2.2
50	1s	49	ILE	2.2
2	2B	17	C	2.2
3	2D	33	LEU	2.2
7	2H	101	ARG	2.2
9	2N	82	LEU	2.2
11	2P	6	LEU	2.2
12	2Q	5	ARG	2.2
14	2S	9	ARG	2.2
32	2a	307	C	2.2
32	2a	1260	C	2.2
42	1k	98	LEU	2.2
55	2x	34	C	2.2
1	2A	2098	U	2.2
1	1A	2805	G	2.2
1	2A	1183	G	2.2
1	2A	2717	G	2.2

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Mol	Chain	Res	Type	RSRZ
2	2B	119	G	2.2
8	2I	85	GLU	2.2
21	1Z	166	SER	2.2
32	1a	98	G	2.2
32	2a	15	G	2.2
32	2a	198	G	2.2
32	2a	987	G	2.2
54	1w	22	G	2.2
55	2x	53	G	2.2
13	2R	69	ASP	2.2
33	2b	199	TYR	2.2
38	1g	18	TYR	2.2
40	1i	110	GLU	2.2
8	2I	37	VAL	2.2
14	1S	65	VAL	2.2
16	1U	100	VAL	2.2
20	2Y	13	VAL	2.2
21	2Z	71	VAL	2.2
35	1d	8	VAL	2.2
42	1k	17	GLY	2.2
16	1U	79	PHE	2.2
35	2d	185	PHE	2.2
9	1N	47	ALA	2.2
18	1W	5	ALA	2.2
34	2c	53	ALA	2.2
36	1e	48	ALA	2.2
36	1e	138	ALA	2.2
45	2n	59	ALA	2.2
1	2A	2418	A	2.2
32	1a	16	A	2.2
32	2a	1092	A	2.2
39	2h	91	ARG	2.2
51	2t	25	ARG	2.2
17	1V	70	ILE	2.2
18	1W	24	ILE	2.2
18	2W	6	ILE	2.2
36	2e	101	ILE	2.2
48	2q	90	ILE	2.2
1	2A	876	C	2.2
3	1D	61	LEU	2.2
8	2I	44	LEU	2.2
9	2N	87	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
13	2R	20	LEU	2.2
32	1a	856	C	2.2
32	1a	1260	C	2.2
33	2b	145	LEU	2.2
34	1c	22	TRP	2.2
35	2d	58	LEU	2.2
35	2d	101	LEU	2.2
36	1e	91	LEU	2.2
43	1l	27	LEU	2.2
48	1q	78	GLU	2.2
9	1N	126	PRO	2.2
24	12	33	MET	2.2
40	1i	98	PRO	2.2
41	2j	86	MET	2.2
37	1f	83	ASP	2.2
51	1t	82	SER	2.2
24	12	42	GLY	2.2
35	2d	116	GLN	2.2
35	2d	180	GLY	2.2
41	2j	33	GLN	2.2
8	2I	89	TYR	2.1
13	2R	21	TYR	2.1
19	1X	69	TYR	2.1
32	1a	148	G	2.1
32	1a	191	G	2.1
32	1a	1068	G	2.1
32	2a	973	G	2.1
32	2a	1120	G	2.1
32	2a	1258	G	2.1
8	1I	37	VAL	2.1
11	2P	90	ARG	2.1
21	1Z	27	VAL	2.1
25	13	47	VAL	2.1
39	1h	93	VAL	2.1
42	1k	105	VAL	2.1
44	2m	117	VAL	2.1
45	2n	19	ARG	2.1
51	2t	73	HIS	2.1
5	1F	167	ALA	2.1
8	1I	55	ALA	2.1
38	2g	147	ALA	2.1
45	2n	48	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
53	2v	19	U	2.1
1	1A	1509(A)	A	2.1
1	2A	2749	A	2.1
3	1D	75	ILE	2.1
12	2Q	127	ILE	2.1
32	1a	1324	A	2.1
32	2a	1225	A	2.1
6	2G	82	LEU	2.1
6	2G	172	LEU	2.1
9	1N	33	LEU	2.1
32	2a	1218	C	2.1
32	2a	1226	C	2.1
40	2i	47	LEU	2.1
51	2t	20	LEU	2.1
9	1N	11	PRO	2.1
4	1E	117	MET	2.1
4	1E	168	MET	2.1
30	28	34	TRP	2.1
38	1g	36	LYS	2.1
43	2l	45	PRO	2.1
17	2V	63	GLY	2.1
19	2X	20	GLY	2.1
31	29	1	MET	2.1
38	1g	34	GLY	2.1
44	2m	95	GLY	2.1
7	1H	132	ARG	2.1
34	1c	38	ARG	2.1
52	2u	6	ARG	2.1
1	2A	10	G	2.1
1	2A	271(M)	G	2.1
1	2A	968	G	2.1
1	2A	2099	U	2.1
4	2E	196	VAL	2.1
9	2N	52	VAL	2.1
14	2S	75	GLU	2.1
32	1a	170	U	2.1
22	20	30	VAL	2.1
32	2a	107	G	2.1
32	2a	1056	U	2.1
44	1m	87	TYR	2.1
48	2q	42	TYR	2.1
28	26	5	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
33	2b	7	VAL	2.1
34	1c	151	VAL	2.1
44	1m	53	VAL	2.1
5	2F	42	ALA	2.1
6	2G	141	PHE	2.1
16	2U	115	ALA	2.1
27	15	2	ALA	2.1
36	1e	95	ALA	2.1
42	1k	69	ALA	2.1
47	1p	56	ALA	2.1
34	2c	4	LYS	2.1
48	2q	87	LYS	2.1
1	2A	228	A	2.1
1	2A	861	A	2.1
1	2A	1029	A	2.1
8	2I	51	ILE	2.1
23	2I	58	ILE	2.1
25	23	43	ILE	2.1
32	2a	782	A	2.1
32	2a	1123	A	2.1
32	2a	1306	A	2.1
46	1o	36	ILE	2.1
3	2D	257	LEU	2.1
13	2R	54	LEU	2.1
17	1V	38	LEU	2.1
2	2B	3	C	2.1
21	2Z	66	SER	2.1
41	2j	85	LEU	2.1
26	14	55	ARG	2.1
29	27	26	GLY	2.1
32	1a	103	C	2.1
32	1a	169	C	2.1
32	2a	620	C	2.1
48	2q	66	SER	2.1
34	1c	96	GLY	2.1
34	2c	80	GLY	2.1
38	2g	19	GLY	2.1
39	1h	128	GLY	2.1
48	1q	91	ARG	2.1
54	2w	3	C	2.1
6	2G	100	TRP	2.1
32	2a	1025	U	2.1

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Mol	Chain	Res	Type	RSRZ
34	2c	167	TRP	2.1
3	2D	113	VAL	2.1
4	1E	165	VAL	2.1
17	2V	92	THR	2.1
20	1Y	15	VAL	2.1
28	26	14	THR	2.1
30	28	14	VAL	2.1
1	2A	614(B)	G	2.1
1	2A	799	G	2.1
6	2G	169	ALA	2.1
10	1O	98	VAL	2.1
39	1h	20	TYR	2.1
40	2i	112	LYS	2.1
41	1j	26	ALA	2.1
45	1n	34	TYR	2.1
7	2H	57	ASP	2.1
16	2U	79	PHE	2.1
32	1a	1186	G	2.1
32	1a	1202	G	2.1
49	2r	73	ALA	2.1
54	1w	29	G	2.1
54	2w	28	G	2.1
16	1U	80	ILE	2.1
16	2U	65	ILE	2.1
28	26	28	ARG	2.1
1	2A	911	A	2.1
3	1D	160	GLY	2.1
4	2E	141	ILE	2.1
4	2E	177	PRO	2.1
8	2I	97	ILE	2.1
33	2b	233	SER	2.1
34	2c	38	ARG	2.1
34	2c	164	ARG	2.1
35	2d	67	ILE	2.1
39	1h	122	ARG	2.1
46	2o	24	SER	2.1
49	1r	42	ARG	2.1
51	1t	23	ARG	2.1
5	2F	33	LEU	2.1
17	1V	40	LEU	2.1
19	1X	9	LEU	2.1
32	1a	1157	A	2.1

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Mol	Chain	Res	Type	RSRZ
32	2a	16	A	2.1
32	2a	1252	A	2.1
44	1m	81	LEU	2.1
45	1n	6	LEU	2.1
46	2o	32	LEU	2.1
51	1t	50	GLU	2.1
51	1t	92	LEU	2.1
1	2A	2507	C	2.1
32	1a	1352	C	2.1
32	2a	84	U	2.1
32	2a	470	C	2.1
26	14	18	CYS	2.1
34	1c	93	LYS	2.1
41	2j	14	LYS	2.1
56	1z	7	CYS	2.1
16	1U	61	TRP	2.1
29	27	40	TRP	2.1
42	1k	42	TRP	2.1
33	2b	110	GLN	2.1
34	2c	170	GLN	2.1
34	2c	183	ASP	2.1
12	2Q	27	VAL	2.1
12	2Q	117	ALA	2.1
16	1U	21	ALA	2.1
17	1V	22	VAL	2.1
18	1W	59	VAL	2.1
18	1W	70	TYR	2.1
19	1X	26	TYR	2.1
21	2Z	165	VAL	2.1
30	18	22	VAL	2.1
33	2b	230	VAL	2.1
34	2c	50	ALA	2.1
34	2c	207	VAL	2.1
35	2d	105	VAL	2.1
38	1g	2	ALA	2.1
48	2q	19	VAL	2.1
28	26	12	GLU	2.1
34	2c	46	GLU	2.1
41	1j	60	ARG	2.1
47	1p	80	PHE	2.1
1	1A	776	G	2.1
1	2A	1169	G	2.1

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Mol	Chain	Res	Type	RSRZ
1	2A	2330	G	2.1
1	2A	2338	G	2.1
32	2a	1155	G	2.1
32	2a	1177	G	2.1
7	1H	117	PRO	2.1
21	2Z	68	PRO	2.1
22	20	76	GLY	2.1
36	2e	44	GLY	2.1
38	1g	77	SER	2.1
48	2q	64	PRO	2.1
3	2D	105	ILE	2.1
50	2s	62	ILE	2.1
16	2U	83	LEU	2.1
22	20	84	LEU	2.1
24	22	10	LEU	2.1
24	22	21	LEU	2.1
33	1b	61	LEU	2.1
34	2c	188	LEU	2.1
41	1j	65	LEU	2.1
1	1A	529	A	2.1
1	2A	918	A	2.1
32	1a	185	A	2.1
32	1a	914	A	2.1
32	2a	900	A	2.1
32	2a	1201	A	2.1
32	2a	1332	A	2.1
1	2A	914	C	2.1
32	1a	221	C	2.1
47	2p	1	MET	2.1
48	2q	29	HIS	2.1
3	2D	250	TRP	2.1
5	1F	39	TRP	2.1
12	2Q	16	ARG	2.1
13	1R	112	ALA	2.1
18	1W	3	ALA	2.1
19	2X	84	ALA	2.1
30	28	17	THR	2.1
33	1b	137	ARG	2.1
45	2n	57	ARG	2.1
41	2j	18	ALA	2.1
44	2m	43	THR	2.1
35	2d	161	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
4	1E	75	VAL	2.1
9	2N	140	VAL	2.1
17	2V	79	VAL	2.1
34	2c	138	VAL	2.1
42	1k	80	VAL	2.1
5	2F	59	TYR	2.1
21	1Z	26	GLY	2.1
35	2d	69	GLY	2.1
35	2d	138	TYR	2.1
36	1e	28	PHE	2.1
38	2g	151	TYR	2.1
45	1n	38	GLY	2.1
45	1n	60	SER	2.1
48	2q	17	LYS	2.1
52	1u	3	LYS	2.1
1	1A	176	G	2.1
1	1A	1042	G	2.1
9	1N	86	PRO	2.1
32	1a	183	G	2.1
32	2a	887	G	2.1
32	2a	1143	G	2.1
32	2a	1305	G	2.1
47	2p	46	PRO	2.1
6	2G	140	ILE	2.1
9	1N	82	LEU	2.1
21	2Z	146	ILE	2.1
23	1l	80	LEU	2.1
51	2t	33	ILE	2.1
8	1I	41	GLU	2.1
1	1A	790	C	2.1
1	1A	1251	C	2.1
1	2A	567	A	2.1
1	2A	837	C	2.1
6	2G	115	ARG	2.1
32	2a	165	C	2.1
32	2a	932	C	2.1
54	2w	38	A	2.1
34	1c	85	ARG	2.1
43	2l	19	ARG	2.1
11	2P	57	THR	2.1
15	1T	59	THR	2.1
40	1i	11	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
41	2j	48	THR	2.1
3	2D	80	ALA	2.1
18	1W	32	ALA	2.1
3	1D	205	VAL	2.1
4	1E	21	VAL	2.1
4	2E	59	VAL	2.1
5	2F	157	VAL	2.1
7	1H	15	VAL	2.1
9	1N	9	VAL	2.1
43	2l	96	VAL	2.1
44	1m	74	VAL	2.1
50	1s	67	VAL	2.1
5	1F	59	TYR	2.1
39	2h	74	PRO	2.1
12	2Q	112	GLU	2.0
1	1A	488	G	2.0
1	2A	2455	G	2.0
7	2H	64	LEU	2.0
9	1N	99	LEU	2.0
9	1N	120	LEU	2.0
12	1Q	2	LEU	2.0
16	1U	109	LEU	2.0
19	1X	8	ILE	2.0
20	2Y	44	ILE	2.0
23	2l	95	LEU	2.0
32	2a	951	G	2.0
32	2a	1310	G	2.0
33	1b	36	ARG	2.0
37	2f	19	LEU	2.0
41	1j	40	LEU	2.0
44	2m	66	LEU	2.0
46	2o	39	LEU	2.0
47	1p	18	ARG	2.0
47	1p	36	ILE	2.0
1	1A	1507	A	2.0
1	1A	2801(A)	A	2.0
1	2A	1204	A	2.0
1	2A	1460	A	2.0
1	2A	1566	A	2.0
1	2A	2742	C	2.0
20	2Y	5	MET	2.0
32	2a	123	C	2.0

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Mol	Chain	Res	Type	RSRZ
33	2b	83	MET	2.0
44	1m	120	LYS	2.0
48	1q	15	MET	2.0
48	2q	100	LYS	2.0
32	2a	889	A	2.0
32	2a	1044	A	2.0
34	2c	98	ASN	2.0
55	1x	56	C	2.0
38	1g	54	THR	2.0
7	2H	146	ALA	2.0
9	2N	92	ALA	2.0
13	2R	62	ALA	2.0
24	22	13	ALA	2.0
25	23	21	ALA	2.0
34	1c	185	GLY	2.0
43	2l	30	ALA	2.0
35	2d	152	SER	2.0
45	2n	28	GLY	2.0
3	1D	241	PRO	2.0
19	1X	29	TRP	2.0
23	11	49	VAL	2.0
39	1h	67	PRO	2.0
43	2l	94	PRO	2.0
46	2o	9	GLN	2.0
35	1d	93	PHE	2.0
39	1h	138	TRP	2.0
47	1p	51	VAL	2.0
48	2q	23	VAL	2.0
3	2D	9	TYR	2.0
4	1E	84	PHE	2.0
4	2E	135	HIS	2.0
8	1I	25	TYR	2.0
18	1W	45	TYR	2.0
25	23	55	ARG	2.0
31	29	22	ARG	2.0
33	2b	8	LYS	2.0
35	1d	22	LYS	2.0
4	1E	27	LEU	2.0
4	1E	49	LEU	2.0
5	1F	28	ILE	2.0
5	2F	32	LEU	2.0
8	2I	109	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
10	2O	2	ILE	2.0
13	2R	111	LEU	2.0
15	2T	50	ILE	2.0
18	1W	29	LEU	2.0
18	2W	86	LEU	2.0
30	28	62	LEU	2.0
35	1d	126	ILE	2.0
44	2m	9	ILE	2.0
51	1t	91	LEU	2.0
1	1A	405	U	2.0
1	1A	919	G	2.0
1	1A	2252	G	2.0
1	2A	7	G	2.0
32	1a	144	G	2.0
32	1a	289	G	2.0
32	2a	1122	U	2.0
48	2q	94	ASN	2.0
55	2x	52	G	2.0
46	2o	59	MET	2.0
1	2A	912	C	2.0
32	2a	369	C	2.0
32	2a	1259	C	2.0
1	2A	631	A	2.0
1	2A	2310	A	2.0
4	1E	24	THR	2.0
7	2H	161	GLY	2.0
8	1I	40	THR	2.0
32	1a	349	A	2.0
32	2a	60	A	2.0
32	2a	162	A	2.0
32	2a	1227	A	2.0
50	2s	27	GLU	2.0
34	1c	191	THR	2.0
53	1v	23	A	2.0
3	1D	93	ALA	2.0
15	2T	31	SER	2.0
16	2U	35	ALA	2.0
31	29	34	GLN	2.0
38	1g	117	ALA	2.0
44	2m	76	ALA	2.0
9	2N	86	PRO	2.0
18	1W	14	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
33	1b	234	PRO	2.0
15	1T	28	VAL	2.0
25	23	50	VAL	2.0
34	1c	26	LYS	2.0
41	2j	49	VAL	2.0
14	1S	12	PHE	2.0
17	1V	81	TYR	2.0
47	2p	38	TYR	2.0
44	1m	86	CYS	2.0
45	1n	27	CYS	2.0
3	2D	133	LEU	2.0
13	1R	4	LEU	2.0
35	2d	5	ILE	2.0
1	1A	1089	G	2.0
1	2A	652(C)	G	2.0
2	2B	86	G	2.0
4	1E	65	GLY	2.0
7	2H	41	MET	2.0
10	1O	50	GLY	2.0
15	1T	1	MET	2.0
32	1a	66	G	2.0
32	1a	944	G	2.0
32	1a	1276	G	2.0
32	2a	1401	G	2.0
33	2b	45	GLN	2.0
37	1f	58	GLY	2.0
1	1A	34	C	2.0
32	1a	224	C	2.0
32	2a	100	C	2.0
32	2a	940	C	2.0
1	2A	819	A	2.0
3	2D	38	LYS	2.0
8	2I	95	LYS	2.0
32	2a	1256	A	2.0
32	2a	1329	A	2.0
35	1d	168	ARG	2.0
41	1j	5	ARG	2.0
41	1j	51	ARG	2.0
42	2k	96	ARG	2.0
14	1S	37	ALA	2.0
17	1V	55	ALA	2.0
18	2W	32	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
44	1m	76	ALA	2.0
54	2w	36	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(Å ²)	Q<0.9
57	4SU	2y	8	20/21	0.49	0.40	87,92,105,113	0
57	5MU	2y	54	21/22	0.58	0.52	74,87,96,109	0
57	G7M	1y	46	24/25	0.62	0.32	78,83,88,95	0
57	G7M	2y	46	24/25	0.65	0.33	83,86,90,104	0
57	PSU	2y	32	20/21	0.66	0.58	78,85,93,95	0
57	MIA	2y	37	22/30	0.67	0.67	79,86,93,107	0
57	PSU	2y	55	20/21	0.67	0.51	82,86,91,100	0
57	MIA	1y	37	22/30	0.70	0.51	73,81,92,101	0
57	PSU	1y	32	20/21	0.70	0.43	75,80,91,93	0
54	G7M	2w	46	24/25	0.70	0.26	72,80,92,108	0
56	FME	1z	1	10/11	0.70	0.53	51,62,66,67	0
57	4SU	1y	8	20/21	0.72	0.38	81,87,95,100	0
57	PSU	1y	39	20/21	0.73	0.51	75,83,86,93	0
57	5MU	1y	54	21/22	0.74	0.47	77,81,87,99	0
57	PSU	1y	55	20/21	0.74	0.54	77,83,88,96	0
57	PSU	2y	39	20/21	0.76	0.48	77,82,90,94	0
54	G7M	1w	46	24/25	0.79	0.20	65,73,89,111	0
56	FME	2z	1	10/11	0.79	0.73	59,67,73,76	0
54	4SU	2w	8	20/21	0.84	0.23	74,79,91,92	0
54	MIA	2w	37	25/30	0.86	0.27	61,67,79,99	0
54	PSU	2w	32	20/21	0.87	0.24	60,71,78,79	0
54	4SU	1w	8	20/21	0.88	0.23	71,75,83,85	0
32	M2G	2a	966	25/26	0.88	0.25	52,60,71,77	0
54	PSU	1w	32	20/21	0.88	0.23	49,57,68,70	0
32	2MG	2a	1207	24/25	0.89	0.22	64,72,75,76	0
55	4SU	2x	8	20/21	0.89	0.17	60,67,72,76	0
43	0TD	2l	92	10/11	0.90	0.21	48,53,61,66	0
54	5MU	2w	54	21/22	0.91	0.18	64,70,73,78	0
54	PSU	1w	55	20/21	0.91	0.19	50,66,71,73	0
54	MIA	1w	37	29/30	0.91	0.27	38,46,64,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	5MC	2a	967	21/22	0.91	0.18	58,61,66,69	0
32	G7M	2a	527	24/25	0.92	0.19	49,56,62,71	0
55	PSU	2x	55	20/21	0.92	0.20	61,66,72,80	0
55	5MC	1x	32	21/22	0.92	0.23	41,46,52,60	0
55	PSU	1x	55	20/21	0.92	0.22	51,58,69,74	0
55	4SU	1x	8	20/21	0.92	0.15	53,59,66,67	0
54	PSU	2w	55	20/21	0.92	0.17	70,74,77,82	0
32	5MC	2a	1404	21/22	0.92	0.21	45,52,55,57	0
1	5MU	2A	1915	21/22	0.92	0.16	51,60,63,66	0
32	UR3	2a	1498	21/22	0.93	0.25	48,51,55,58	0
43	0TD	1l	92	10/11	0.93	0.22	40,46,48,56	0
1	5MU	1A	1915	21/22	0.93	0.17	33,44,48,50	0
32	2MG	1a	1207	24/25	0.93	0.17	50,55,58,69	0
1	PSU	2A	1917	20/21	0.93	0.15	51,56,66,70	0
32	PSU	2a	516	20/21	0.93	0.17	57,63,67,73	0
55	5MU	2x	54	21/22	0.94	0.26	67,72,77,80	0
32	MA6	1a	1519	24/25	0.94	0.22	35,39,45,53	0
1	PSU	2A	1911	20/21	0.94	0.16	50,57,60,64	0
55	5MU	1x	54	21/22	0.94	0.20	58,63,71,76	0
54	PSU	2w	39	20/21	0.94	0.23	62,70,75,76	0
32	5MC	2a	1400	21/22	0.94	0.25	54,59,65,69	0
32	4OC	2a	1402	22/23	0.94	0.18	48,52,56,57	0
32	M2G	1a	966	25/26	0.94	0.21	41,48,51,52	0
32	5MC	2a	1407	21/22	0.94	0.18	40,47,51,60	0
1	OMU	2A	2552	21/22	0.94	0.23	31,41,45,49	0
55	8AN	1x	76	22/23	0.94	0.23	22,26,32,39	0
32	PSU	1a	516	20/21	0.94	0.18	44,48,52,53	0
55	5MC	2x	32	21/22	0.95	0.18	57,60,66,72	0
1	PSU	1A	1917	20/21	0.95	0.18	36,42,48,52	0
1	OMC	2A	1920	21/22	0.95	0.16	44,53,56,57	0
1	5MC	2A	1942	21/22	0.95	0.17	40,51,54,57	0
54	PSU	1w	39	20/21	0.95	0.23	41,57,62,65	0
1	5MC	2A	1962	21/22	0.95	0.18	36,43,49,58	0
32	4OC	1a	1402	22/23	0.95	0.21	33,40,44,46	0
1	PSU	2A	2605	20/21	0.95	0.20	30,36,40,45	0
54	5MU	1w	54	21/22	0.95	0.17	50,57,62,66	0
32	5MC	1a	1404	21/22	0.95	0.19	32,38,41,45	0
32	MA6	2a	1518	24/25	0.95	0.21	46,55,60,62	0
32	MA6	2a	1519	24/25	0.95	0.24	41,55,60,61	0
32	5MC	1a	1407	21/22	0.95	0.19	29,36,42,44	0
32	5MC	1a	967	21/22	0.95	0.22	43,51,56,57	0
32	G7M	1a	527	24/25	0.96	0.19	35,41,47,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	OMC	1A	1920	21/22	0.96	0.20	33,40,45,49	0
32	UR3	1a	1498	21/22	0.96	0.21	32,39,40,44	0
55	8AN	2x	76	22/23	0.96	0.19	29,37,40,47	0
32	MA6	1a	1518	24/25	0.96	0.21	31,40,43,44	0
1	5MU	1A	1939	21/22	0.96	0.20	21,25,29,30	0
1	5MC	1A	1942	21/22	0.96	0.20	28,37,47,51	0
32	5MC	1a	1400	21/22	0.96	0.19	37,40,44,46	0
1	PSU	1A	1911	20/21	0.96	0.17	37,43,47,49	0
1	5MC	1A	1962	21/22	0.97	0.20	25,31,37,40	0
1	5MU	2A	1939	21/22	0.97	0.20	30,36,39,42	0
1	2MA	1A	2503	23/24	0.97	0.22	16,21,27,27	0
1	OMU	1A	2552	21/22	0.97	0.17	20,25,30,30	0
54	F3N	1w	76	33/34	0.97	0.23	16,23,26,28	0
54	F3N	2w	76	33/34	0.97	0.21	23,37,41,41	0
1	2MA	2A	2503	23/24	0.97	0.19	25,33,39,41	0
1	PSU	1A	2605	20/21	0.97	0.19	19,26,30,32	0
1	OMG	1A	2251	24/25	0.98	0.20	18,25,29,32	0
1	OMG	2A	2251	24/25	0.98	0.22	34,38,41,43	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2a	1712	1/1	0.14	0.24	75,75,75,75	0
58	MG	1x	105	1/1	0.19	0.22	62,62,62,62	0
58	MG	2a	1635	1/1	0.21	0.33	64,64,64,64	0
58	MG	2a	1640	1/1	0.23	0.41	74,74,74,74	0
58	MG	2a	1637	1/1	0.23	0.19	78,78,78,78	0
58	MG	2a	1672	1/1	0.25	0.21	69,69,69,69	0
58	MG	2A	3160	1/1	0.26	0.51	66,66,66,66	0
58	MG	2a	1724	1/1	0.27	0.28	75,75,75,75	0
58	MG	2A	3280	1/1	0.32	0.21	58,58,58,58	0
58	MG	2A	3174	1/1	0.35	0.17	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	1805	1/1	0.37	0.21	70,70,70,70	0
58	MG	1A	3541	1/1	0.38	0.23	48,48,48,48	0
58	MG	2A	3307	1/1	0.38	0.21	65,65,65,65	0
58	MG	2A	3242	1/1	0.38	0.26	57,57,57,57	0
58	MG	2a	1709	1/1	0.39	0.23	69,69,69,69	0
58	MG	2a	1820	1/1	0.39	0.22	68,68,68,68	0
58	MG	1a	1758	1/1	0.40	0.11	67,67,67,67	0
58	MG	1A	3204	1/1	0.41	0.19	58,58,58,58	0
58	MG	1A	3946	1/1	0.41	0.16	71,71,71,71	0
58	MG	1A	3924	1/1	0.42	0.16	64,64,64,64	0
58	MG	1a	1615	1/1	0.43	0.17	58,58,58,58	0
58	MG	2a	1651	1/1	0.43	0.23	71,71,71,71	0
58	MG	2A	3293	1/1	0.44	0.48	68,68,68,68	0
58	MG	1A	3559	1/1	0.44	0.25	72,72,72,72	0
58	MG	1A	3542	1/1	0.45	0.19	60,60,60,60	0
58	MG	2A	3455	1/1	0.45	0.29	59,59,59,59	0
58	MG	2n	101	1/1	0.45	0.31	77,77,77,77	0
58	MG	1A	4066	1/1	0.46	0.16	59,59,59,59	0
58	MG	1a	1642	1/1	0.46	0.39	55,55,55,55	0
58	MG	2A	3156	1/1	0.46	0.25	70,70,70,70	0
58	MG	2A	3374	1/1	0.46	0.23	66,66,66,66	0
58	MG	2A	3332	1/1	0.47	0.26	56,56,56,56	0
58	MG	2a	1634	1/1	0.48	0.33	58,58,58,58	0
58	MG	2A	3389	1/1	0.48	0.37	69,69,69,69	0
58	MG	1A	3537	1/1	0.48	0.26	64,64,64,64	0
58	MG	2A	3082	1/1	0.49	0.24	51,51,51,51	0
58	MG	2A	3272	1/1	0.49	0.28	70,70,70,70	0
58	MG	1A	3887	1/1	0.49	0.20	57,57,57,57	0
58	MG	20	101	1/1	0.49	0.43	69,69,69,69	0
58	MG	2A	3238	1/1	0.50	0.27	60,60,60,60	0
58	MG	1A	4035	1/1	0.50	0.23	53,53,53,53	0
58	MG	2a	1739	1/1	0.50	0.24	51,51,51,51	0
58	MG	1A	3333	1/1	0.51	0.28	45,45,45,45	0
58	MG	2A	3253	1/1	0.51	0.26	74,74,74,74	0
58	MG	2A	3212	1/1	0.51	0.17	66,66,66,66	0
58	MG	2A	3116	1/1	0.51	0.21	53,53,53,53	0
58	MG	1A	3519	1/1	0.52	0.32	70,70,70,70	0
58	MG	2A	3040	1/1	0.52	0.24	64,64,64,64	0
58	MG	2a	1744	1/1	0.52	0.16	81,81,81,81	0
58	MG	2a	1605	1/1	0.53	0.19	69,69,69,69	0
58	MG	1A	3410	1/1	0.53	0.21	64,64,64,64	0
58	MG	1x	109	1/1	0.53	0.22	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2a	1808	1/1	0.53	0.23	70,70,70,70	0
58	MG	2A	3648	1/1	0.53	0.11	68,68,68,68	0
58	MG	1A	3270	1/1	0.53	0.23	64,64,64,64	0
58	MG	1a	1742	1/1	0.54	1.17	80,80,80,80	0
58	MG	1A	3343	1/1	0.54	0.19	56,56,56,56	0
58	MG	1A	3942	1/1	0.55	0.30	67,67,67,67	0
58	MG	1A	3871	1/1	0.55	0.19	52,52,52,52	0
58	MG	2R	204	1/1	0.55	0.42	65,65,65,65	0
58	MG	1a	1659	1/1	0.55	0.20	68,68,68,68	0
58	MG	2v	103	1/1	0.55	0.17	79,79,79,79	0
58	MG	2A	3315	1/1	0.56	0.22	68,68,68,68	0
58	MG	1A	4026	1/1	0.56	0.26	58,58,58,58	0
58	MG	1A	3563	1/1	0.56	0.28	46,46,46,46	0
58	MG	1a	1791	1/1	0.56	0.11	59,59,59,59	0
58	MG	2a	1619	1/1	0.56	0.20	61,61,61,61	0
58	MG	2A	3407	1/1	0.56	0.24	51,51,51,51	0
58	MG	1a	1798	1/1	0.56	0.11	57,57,57,57	0
58	MG	2w	103	1/1	0.56	0.29	74,74,74,74	0
58	MG	2a	1649	1/1	0.57	0.19	74,74,74,74	0
58	MG	1A	3128	1/1	0.57	0.19	53,53,53,53	0
58	MG	2A	3610	1/1	0.57	0.18	62,62,62,62	0
58	MG	1A	3592	1/1	0.57	0.20	66,66,66,66	0
58	MG	2A	3792	1/1	0.57	0.16	46,46,46,46	0
58	MG	1w	103	1/1	0.57	0.18	72,72,72,72	0
58	MG	1A	3351	1/1	0.57	0.49	59,59,59,59	0
58	MG	1a	1808	1/1	0.58	0.19	78,78,78,78	0
58	MG	2A	3803	1/1	0.58	0.21	56,56,56,56	0
58	MG	2A	3813	1/1	0.58	0.20	45,45,45,45	0
58	MG	2D	307	1/1	0.58	0.28	67,67,67,67	0
58	MG	1A	4031	1/1	0.58	0.12	49,49,49,49	0
58	MG	2A	3255	1/1	0.58	0.21	60,60,60,60	0
58	MG	2A	3388	1/1	0.58	0.30	64,64,64,64	0
58	MG	2A	3197	1/1	0.58	0.44	67,67,67,67	0
58	MG	2A	3203	1/1	0.58	0.21	70,70,70,70	0
58	MG	2A	3413	1/1	0.58	0.18	60,60,60,60	0
58	MG	2A	3289	1/1	0.58	0.48	58,58,58,58	0
58	MG	1B	224	1/1	0.58	0.27	61,61,61,61	0
58	MG	1A	3429	1/1	0.58	0.17	62,62,62,62	0
58	MG	1Y	203	1/1	0.59	0.23	67,67,67,67	0
58	MG	1A	4002	1/1	0.59	0.11	57,57,57,57	0
58	MG	2D	302	1/1	0.59	0.32	56,56,56,56	0
58	MG	1a	1622	1/1	0.59	0.21	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	1628	1/1	0.59	0.22	59,59,59,59	0
58	MG	2T	203	1/1	0.59	0.20	62,62,62,62	0
58	MG	2A	3355	1/1	0.59	0.18	62,62,62,62	0
58	MG	2A	3281	1/1	0.59	0.18	60,60,60,60	0
58	MG	1A	3486	1/1	0.59	0.31	58,58,58,58	0
58	MG	2A	3807	1/1	0.60	0.09	63,63,63,63	0
58	MG	2a	1729	1/1	0.60	0.16	61,61,61,61	0
58	MG	2A	3309	1/1	0.60	0.22	52,52,52,52	0
58	MG	1A	3264	1/1	0.60	0.19	53,53,53,53	0
58	MG	2A	3448	1/1	0.60	0.19	68,68,68,68	0
58	MG	1A	3369	1/1	0.60	0.29	49,49,49,49	0
58	MG	1A	3793	1/1	0.60	0.12	36,36,36,36	0
58	MG	2A	3168	1/1	0.60	0.15	52,52,52,52	0
58	MG	1A	4061	1/1	0.60	0.18	48,48,48,48	0
58	MG	1a	1704	1/1	0.60	0.19	66,66,66,66	0
58	MG	1a	1690	1/1	0.61	0.20	60,60,60,60	0
58	MG	1A	3719	1/1	0.61	0.31	64,64,64,64	0
58	MG	2A	3166	1/1	0.61	0.20	60,60,60,60	0
58	MG	1A	3957	1/1	0.61	0.10	58,58,58,58	0
58	MG	1A	3976	1/1	0.61	0.41	65,65,65,65	0
58	MG	1a	1784	1/1	0.61	0.10	52,52,52,52	0
58	MG	1A	3439	1/1	0.61	0.22	66,66,66,66	0
58	MG	2A	3748	1/1	0.61	0.17	54,54,54,54	0
58	MG	2a	1602	1/1	0.61	0.15	67,67,67,67	0
58	MG	1a	1687	1/1	0.61	0.25	53,53,53,53	0
58	MG	10	107	1/1	0.62	0.31	67,67,67,67	0
58	MG	1a	1606	1/1	0.62	0.38	52,52,52,52	0
58	MG	2V	202	1/1	0.62	0.27	68,68,68,68	0
58	MG	2A	3824	1/1	0.62	0.27	73,73,73,73	0
58	MG	2A	3826	1/1	0.62	0.18	61,61,61,61	0
58	MG	1A	3962	1/1	0.62	0.13	58,58,58,58	0
58	MG	1A	3423	1/1	0.62	0.24	59,59,59,59	0
58	MG	2q	201	1/1	0.62	0.15	60,60,60,60	0
58	MG	2a	1624	1/1	0.62	0.20	60,60,60,60	0
58	MG	2E	304	1/1	0.62	0.18	65,65,65,65	0
58	MG	1A	3342	1/1	0.63	0.25	57,57,57,57	0
58	MG	2A	3730	1/1	0.63	0.24	70,70,70,70	0
58	MG	2A	3234	1/1	0.63	0.19	63,63,63,63	0
58	MG	2A	3131	1/1	0.63	0.17	72,72,72,72	0
58	MG	2A	3136	1/1	0.63	0.23	50,50,50,50	0
58	MG	1A	3245	1/1	0.63	0.36	56,56,56,56	0
58	MG	2A	3596	1/1	0.63	0.17	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	1A	3698	1/1	0.63	0.20	67,67,67,67	0
58	MG	1a	1769	1/1	0.64	0.22	62,62,62,62	0
58	MG	2A	3015	1/1	0.64	0.29	62,62,62,62	0
58	MG	1A	3453	1/1	0.64	0.37	67,67,67,67	0
58	MG	2A	3702	1/1	0.64	0.14	41,41,41,41	0
58	MG	2A	3714	1/1	0.64	0.23	53,53,53,53	0
58	MG	1a	1694	1/1	0.64	0.22	71,71,71,71	0
58	MG	1A	3947	1/1	0.64	0.58	69,69,69,69	0
58	MG	1a	1717	1/1	0.64	0.24	59,59,59,59	0
58	MG	2A	3799	1/1	0.64	0.14	34,34,34,34	0
58	MG	1A	3300	1/1	0.64	0.38	62,62,62,62	0
58	MG	2A	3300	1/1	0.64	0.14	69,69,69,69	0
58	MG	1x	104	1/1	0.64	0.17	60,60,60,60	0
58	MG	1A	4059	1/1	0.64	0.24	56,56,56,56	0
58	MG	2A	3458	1/1	0.64	0.17	69,69,69,69	0
58	MG	2A	3575	1/1	0.64	0.16	43,43,43,43	0
58	MG	2A	3418	1/1	0.65	0.16	67,67,67,67	0
58	MG	1A	3955	1/1	0.65	0.14	48,48,48,48	0
58	MG	2a	1700	1/1	0.65	0.25	80,80,80,80	0
58	MG	2A	3333	1/1	0.65	0.38	50,50,50,50	0
58	MG	1A	3263	1/1	0.65	0.12	57,57,57,57	0
58	MG	2A	3472	1/1	0.65	0.14	56,56,56,56	0
58	MG	1B	228	1/1	0.65	0.30	63,63,63,63	0
58	MG	2A	3384	1/1	0.65	0.51	68,68,68,68	0
58	MG	2A	3814	1/1	0.65	0.14	56,56,56,56	0
58	MG	2A	3816	1/1	0.65	0.14	51,51,51,51	0
58	MG	2a	1629	1/1	0.65	0.18	52,52,52,52	0
58	MG	2A	3218	1/1	0.65	0.27	51,51,51,51	0
58	MG	2A	3137	1/1	0.65	0.21	66,66,66,66	0
58	MG	2A	3837	1/1	0.65	0.42	72,72,72,72	0
58	MG	2A	3144	1/1	0.65	0.18	66,66,66,66	0
58	MG	2A	3321	1/1	0.65	0.19	70,70,70,70	0
58	MG	1A	4020	1/1	0.66	0.09	52,52,52,52	0
58	MG	1a	1693	1/1	0.66	0.25	61,61,61,61	0
58	MG	1a	1619	1/1	0.66	0.26	50,50,50,50	0
58	MG	1A	3006	1/1	0.66	0.22	66,66,66,66	0
58	MG	1a	1623	1/1	0.66	0.18	56,56,56,56	0
58	MG	2A	3541	1/1	0.66	0.21	45,45,45,45	0
58	MG	1A	3409	1/1	0.66	0.64	73,73,73,73	0
58	MG	1A	3356	1/1	0.66	0.32	59,59,59,59	0
58	MG	2A	3349	1/1	0.66	0.32	61,61,61,61	0
58	MG	2A	3618	1/1	0.66	0.14	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1x	110	1/1	0.66	0.14	62,62,62,62	0
58	MG	2A	3356	1/1	0.66	0.16	58,58,58,58	0
58	MG	2A	3165	1/1	0.66	0.20	60,60,60,60	0
58	MG	1x	111	1/1	0.66	0.24	60,60,60,60	0
58	MG	1A	3838	1/1	0.66	0.30	80,80,80,80	0
58	MG	2A	3787	1/1	0.66	0.13	57,57,57,57	0
58	MG	2A	3037	1/1	0.66	0.18	62,62,62,62	0
58	MG	2A	3793	1/1	0.66	0.13	46,46,46,46	0
58	MG	1A	3606	1/1	0.66	0.14	54,54,54,54	0
58	MG	2A	3296	1/1	0.66	0.44	40,40,40,40	0
58	MG	1A	3017	1/1	0.67	0.22	59,59,59,59	0
58	MG	1a	1640	1/1	0.67	0.22	59,59,59,59	0
58	MG	2A	3224	1/1	0.67	0.20	60,60,60,60	0
58	MG	2A	3169	1/1	0.67	0.19	73,73,73,73	0
58	MG	2A	3692	1/1	0.67	0.14	55,55,55,55	0
58	MG	2A	3815	1/1	0.67	0.14	44,44,44,44	0
58	MG	2A	3336	1/1	0.67	0.28	49,49,49,49	0
58	MG	1A	3742	1/1	0.67	0.12	50,50,50,50	0
58	MG	1a	1601	1/1	0.67	0.18	56,56,56,56	0
58	MG	2A	3252	1/1	0.67	0.22	61,61,61,61	0
58	MG	2A	3758	1/1	0.67	0.13	64,64,64,64	0
58	MG	2A	3368	1/1	0.67	0.22	68,68,68,68	0
58	MG	1A	3252	1/1	0.67	0.29	67,67,67,67	0
58	MG	2a	1650	1/1	0.67	0.20	63,63,63,63	0
58	MG	2A	3211	1/1	0.67	0.30	58,58,58,58	0
58	MG	1a	1679	1/1	0.68	0.23	62,62,62,62	0
58	MG	2A	3096	1/1	0.68	0.29	66,66,66,66	0
58	MG	2a	1721	1/1	0.68	0.21	70,70,70,70	0
58	MG	2A	3325	1/1	0.68	0.12	67,67,67,67	0
58	MG	2B	202	1/1	0.68	0.51	59,59,59,59	0
58	MG	2A	3108	1/1	0.68	0.25	64,64,64,64	0
58	MG	1Z	302	1/1	0.68	0.32	57,57,57,57	0
58	MG	2a	1794	1/1	0.68	0.12	68,68,68,68	0
58	MG	1a	1688	1/1	0.68	0.12	61,61,61,61	0
58	MG	2F	301	1/1	0.68	0.24	65,65,65,65	0
58	MG	2A	3345	1/1	0.68	0.26	57,57,57,57	0
58	MG	1A	4022	1/1	0.68	0.20	65,65,65,65	0
58	MG	2A	3021	1/1	0.68	0.20	69,69,69,69	0
58	MG	1R	204	1/1	0.68	0.38	53,53,53,53	0
58	MG	1A	4048	1/1	0.68	0.11	54,54,54,54	0
58	MG	2A	3777	1/1	0.69	0.55	61,61,61,61	0
58	MG	1A	3080	1/1	0.69	0.23	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3488	1/1	0.69	0.25	62,62,62,62	0
58	MG	2A	3237	1/1	0.69	0.15	70,70,70,70	0
58	MG	1A	3413	1/1	0.69	0.15	60,60,60,60	0
58	MG	1a	1691	1/1	0.69	0.13	49,49,49,49	0
58	MG	1A	3158	1/1	0.69	0.21	50,50,50,50	0
58	MG	2a	1638	1/1	0.69	0.23	68,68,68,68	0
58	MG	1A	3669	1/1	0.69	0.16	47,47,47,47	0
58	MG	2a	1804	1/1	0.69	0.37	64,64,64,64	0
58	MG	2a	1641	1/1	0.69	0.17	50,50,50,50	0
58	MG	2a	1648	1/1	0.69	0.26	61,61,61,61	0
58	MG	1A	3475	1/1	0.69	0.34	53,53,53,53	0
58	MG	2A	3471	1/1	0.69	0.15	50,50,50,50	0
58	MG	1A	3482	1/1	0.69	0.32	74,74,74,74	0
58	MG	1A	3740	1/1	0.69	0.12	51,51,51,51	0
58	MG	2a	1677	1/1	0.69	0.15	56,56,56,56	0
58	MG	2a	1681	1/1	0.70	0.19	67,67,67,67	0
58	MG	2a	1698	1/1	0.70	0.17	70,70,70,70	0
58	MG	1A	3966	1/1	0.70	0.25	51,51,51,51	0
58	MG	1a	1734	1/1	0.70	0.28	69,69,69,69	0
58	MG	2A	3683	1/1	0.70	0.18	68,68,68,68	0
58	MG	2A	3233	1/1	0.70	0.26	63,63,63,63	0
58	MG	1a	1741	1/1	0.70	0.15	68,68,68,68	0
58	MG	2A	3447	1/1	0.70	0.23	48,48,48,48	0
58	MG	1A	3378	1/1	0.70	0.20	39,39,39,39	0
58	MG	1A	4029	1/1	0.70	0.17	42,42,42,42	0
58	MG	2a	1758	1/1	0.70	0.11	66,66,66,66	0
58	MG	1a	1764	1/1	0.70	0.15	59,59,59,59	0
58	MG	2A	3469	1/1	0.70	0.15	75,75,75,75	0
58	MG	2A	3358	1/1	0.70	0.21	52,52,52,52	0
58	MG	2a	1807	1/1	0.70	0.32	70,70,70,70	0
58	MG	1A	3721	1/1	0.70	0.32	66,66,66,66	0
58	MG	1Z	303	1/1	0.70	0.22	58,58,58,58	0
58	MG	2d	303	1/1	0.70	0.35	68,68,68,68	0
58	MG	2A	3380	1/1	0.70	0.16	53,53,53,53	0
58	MG	1a	1697	1/1	0.70	0.15	66,66,66,66	0
58	MG	1A	3207	1/1	0.70	0.18	69,69,69,69	0
58	MG	2a	1601	1/1	0.70	0.17	69,69,69,69	0
58	MG	2A	3484	1/1	0.71	0.23	66,66,66,66	0
58	MG	2A	3209	1/1	0.71	0.30	62,62,62,62	0
58	MG	2P	201	1/1	0.71	0.19	58,58,58,58	0
58	MG	1a	1682	1/1	0.71	0.12	71,71,71,71	0
58	MG	2A	3382	1/1	0.71	0.16	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2a	1740	1/1	0.71	0.27	63,63,63,63	0
58	MG	2a	1643	1/1	0.71	0.16	61,61,61,61	0
58	MG	1a	1743	1/1	0.71	0.14	54,54,54,54	0
58	MG	2A	3822	1/1	0.71	0.10	63,63,63,63	0
58	MG	25	103	1/1	0.71	0.42	65,65,65,65	0
58	MG	2A	3617	1/1	0.71	0.17	60,60,60,60	0
58	MG	2a	1653	1/1	0.71	0.35	55,55,55,55	0
58	MG	1a	1770	1/1	0.71	0.12	62,62,62,62	0
58	MG	2A	3222	1/1	0.71	0.32	58,58,58,58	0
58	MG	2A	3665	1/1	0.71	0.23	61,61,61,61	0
58	MG	2B	216	1/1	0.71	0.22	65,65,65,65	0
58	MG	1A	3762	1/1	0.71	0.21	49,49,49,49	0
58	MG	2a	1702	1/1	0.71	0.32	68,68,68,68	0
58	MG	2w	102	1/1	0.71	0.12	62,62,62,62	0
58	MG	1a	1786	1/1	0.71	0.09	59,59,59,59	0
58	MG	2a	1628	1/1	0.72	0.19	65,65,65,65	0
58	MG	2A	3257	1/1	0.72	0.40	69,69,69,69	0
58	MG	2A	3213	1/1	0.72	0.34	36,36,36,36	0
58	MG	2a	1715	1/1	0.72	0.19	65,65,65,65	0
58	MG	2A	3406	1/1	0.72	0.29	61,61,61,61	0
58	MG	2A	3788	1/1	0.72	0.14	60,60,60,60	0
58	MG	2E	301	1/1	0.72	0.21	56,56,56,56	0
58	MG	1A	3401	1/1	0.72	0.23	41,41,41,41	0
58	MG	1A	3956	1/1	0.72	0.40	45,45,45,45	0
58	MG	1A	3743	1/1	0.72	0.15	46,46,46,46	0
58	MG	2A	3640	1/1	0.72	0.70	59,59,59,59	0
58	MG	18	106	1/1	0.72	0.18	55,55,55,55	0
58	MG	1A	3442	1/1	0.72	0.39	54,54,54,54	0
58	MG	2A	3670	1/1	0.72	0.21	66,66,66,66	0
58	MG	2a	1652	1/1	0.72	0.11	72,72,72,72	0
58	MG	1A	3548	1/1	0.72	0.17	64,64,64,64	0
58	MG	2a	1810	1/1	0.72	0.19	79,79,79,79	0
58	MG	2a	1665	1/1	0.72	0.19	63,63,63,63	0
58	MG	1a	1768	1/1	0.72	0.21	62,62,62,62	0
58	MG	1a	1671	1/1	0.72	0.11	73,73,73,73	0
58	MG	1A	3184	1/1	0.72	0.23	38,38,38,38	0
58	MG	2a	1683	1/1	0.72	0.29	57,57,57,57	0
58	MG	1a	1708	1/1	0.72	0.30	63,63,63,63	0
58	MG	1A	3840	1/1	0.72	0.13	37,37,37,37	0
58	MG	2A	3181	1/1	0.73	0.17	61,61,61,61	0
58	MG	1a	1752	1/1	0.73	0.17	67,67,67,67	0
58	MG	2A	3439	1/1	0.73	0.20	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3752	1/1	0.73	0.15	55,55,55,55	0
58	MG	2A	3689	1/1	0.73	0.20	74,74,74,74	0
58	MG	1A	3143	1/1	0.73	0.35	51,51,51,51	0
58	MG	2A	3029	1/1	0.73	0.20	53,53,53,53	0
58	MG	1A	3561	1/1	0.73	0.23	38,38,38,38	0
58	MG	2A	3038	1/1	0.73	0.30	54,54,54,54	0
58	MG	2A	3744	1/1	0.73	0.14	61,61,61,61	0
58	MG	2a	1749	1/1	0.73	0.15	77,77,77,77	0
58	MG	1A	3535	1/1	0.73	0.21	52,52,52,52	0
58	MG	2a	1759	1/1	0.73	0.10	63,63,63,63	0
58	MG	2A	3161	1/1	0.73	0.14	60,60,60,60	0
58	MG	2a	1803	1/1	0.73	0.14	52,52,52,52	0
58	MG	2A	3050	1/1	0.73	0.21	58,58,58,58	0
58	MG	2A	3225	1/1	0.73	0.15	64,64,64,64	0
58	MG	2A	3561	1/1	0.73	0.17	59,59,59,59	0
58	MG	2A	3079	1/1	0.73	0.12	59,59,59,59	0
58	MG	1A	3517	1/1	0.73	0.22	61,61,61,61	0
58	MG	2A	3609	1/1	0.73	0.18	38,38,38,38	0
58	MG	2a	1676	1/1	0.73	0.17	57,57,57,57	0
58	MG	2A	3801	1/1	0.73	0.22	49,49,49,49	0
58	MG	1a	1645	1/1	0.73	0.14	55,55,55,55	0
58	MG	1a	1746	1/1	0.73	0.09	57,57,57,57	0
58	MG	2A	3322	1/1	0.73	0.18	73,73,73,73	0
58	MG	2A	3175	1/1	0.73	0.26	59,59,59,59	0
58	MG	1A	3250	1/1	0.74	0.13	57,57,57,57	0
58	MG	2B	220	1/1	0.74	0.12	69,69,69,69	0
58	MG	2A	3286	1/1	0.74	0.33	65,65,65,65	0
58	MG	1A	3985	1/1	0.74	0.16	42,42,42,42	0
58	MG	1A	3772	1/1	0.74	0.20	29,29,29,29	0
58	MG	2E	302	1/1	0.74	0.16	71,71,71,71	0
58	MG	2a	1696	1/1	0.74	0.18	69,69,69,69	0
58	MG	1A	4075	1/1	0.74	0.23	53,53,53,53	0
58	MG	1A	4087	1/1	0.74	0.12	78,78,78,78	0
58	MG	1a	1621	1/1	0.74	0.21	58,58,58,58	0
58	MG	2A	3747	1/1	0.74	0.14	68,68,68,68	0
58	MG	2A	3128	1/1	0.74	0.16	51,51,51,51	0
58	MG	1B	223	1/1	0.74	0.28	65,65,65,65	0
58	MG	2A	3770	1/1	0.74	0.21	60,60,60,60	0
58	MG	2A	3773	1/1	0.74	0.13	60,60,60,60	0
58	MG	1A	3291	1/1	0.74	0.14	52,52,52,52	0
58	MG	2A	3782	1/1	0.74	0.25	62,62,62,62	0
58	MG	2A	3463	1/1	0.74	0.15	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	2a	1742	1/1	0.74	0.13	55,55,55,55	0
58	MG	2a	1608	1/1	0.74	0.11	67,67,67,67	0
58	MG	1A	3949	1/1	0.74	0.15	45,45,45,45	0
58	MG	1a	1636	1/1	0.74	0.16	53,53,53,53	0
58	MG	1a	1712	1/1	0.74	0.11	61,61,61,61	0
58	MG	2a	1775	1/1	0.74	0.10	62,62,62,62	0
58	MG	1a	1639	1/1	0.74	0.12	65,65,65,65	0
58	MG	1A	3603	1/1	0.74	0.33	66,66,66,66	0
58	MG	1A	3406	1/1	0.74	0.57	44,44,44,44	0
58	MG	2A	3245	1/1	0.74	0.21	49,49,49,49	0
58	MG	2A	3251	1/1	0.74	0.12	63,63,63,63	0
58	MG	1a	1643	1/1	0.74	0.15	56,56,56,56	0
58	MG	1A	3618	1/1	0.74	0.21	39,39,39,39	0
58	MG	1A	3076	1/1	0.74	0.19	27,27,27,27	0
58	MG	1a	1669	1/1	0.74	0.22	56,56,56,56	0
58	MG	2l	203	1/1	0.74	0.12	57,57,57,57	0
58	MG	2A	3270	1/1	0.74	0.20	58,58,58,58	0
58	MG	1A	3695	1/1	0.74	0.17	35,35,35,35	0
58	MG	2A	3279	1/1	0.74	0.15	49,49,49,49	0
58	MG	10	108	1/1	0.74	0.22	64,64,64,64	0
58	MG	2B	205	1/1	0.74	0.10	59,59,59,59	0
58	MG	2A	3637	1/1	0.75	0.18	46,46,46,46	0
58	MG	1A	3633	1/1	0.75	0.16	57,57,57,57	0
58	MG	1A	3568	1/1	0.75	0.37	59,59,59,59	0
58	MG	1A	3299	1/1	0.75	0.23	49,49,49,49	0
58	MG	2a	1748	1/1	0.75	0.24	63,63,63,63	0
58	MG	2A	3005	1/1	0.75	0.16	54,54,54,54	0
58	MG	2a	1753	1/1	0.75	0.21	77,77,77,77	0
58	MG	2A	3135	1/1	0.75	0.25	50,50,50,50	0
58	MG	1D	313	1/1	0.75	0.19	40,40,40,40	0
58	MG	1O	201	1/1	0.75	1.06	65,65,65,65	0
58	MG	2a	1793	1/1	0.75	0.15	75,75,75,75	0
58	MG	1A	3284	1/1	0.75	0.30	52,52,52,52	0
58	MG	2A	3519	1/1	0.75	0.15	49,49,49,49	0
58	MG	1a	1795	1/1	0.75	0.16	65,65,65,65	0
58	MG	2A	3324	1/1	0.75	0.21	60,60,60,60	0
58	MG	2A	3825	1/1	0.75	0.07	52,52,52,52	0
58	MG	1a	1617	1/1	0.75	0.15	41,41,41,41	0
58	MG	2A	3580	1/1	0.75	0.26	62,62,62,62	0
58	MG	2A	3587	1/1	0.75	0.16	62,62,62,62	0
58	MG	1a	1803	1/1	0.75	0.23	72,72,72,72	0
58	MG	2B	208	1/1	0.75	0.16	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3315	1/1	0.75	0.21	59,59,59,59	0
58	MG	1A	3344	1/1	0.75	0.36	64,64,64,64	0
58	MG	2A	3615	1/1	0.75	0.20	63,63,63,63	0
58	MG	1a	1663	1/1	0.75	0.13	58,58,58,58	0
58	MG	1B	212	1/1	0.75	0.34	58,58,58,58	0
58	MG	1A	3435	1/1	0.76	0.15	42,42,42,42	0
58	MG	2A	3481	1/1	0.76	0.23	66,66,66,66	0
58	MG	1a	1692	1/1	0.76	0.15	51,51,51,51	0
58	MG	2A	3676	1/1	0.76	0.11	40,40,40,40	0
58	MG	2a	1751	1/1	0.76	0.13	64,64,64,64	0
58	MG	1a	1774	1/1	0.76	0.10	56,56,56,56	0
58	MG	2a	1755	1/1	0.76	0.14	41,41,41,41	0
58	MG	2A	3540	1/1	0.76	0.20	48,48,48,48	0
58	MG	2A	3403	1/1	0.76	0.19	46,46,46,46	0
58	MG	2A	3241	1/1	0.76	0.32	72,72,72,72	0
58	MG	2A	3712	1/1	0.76	0.27	66,66,66,66	0
58	MG	1A	3392	1/1	0.76	0.25	37,37,37,37	0
58	MG	1a	1678	1/1	0.76	0.16	65,65,65,65	0
58	MG	2A	3733	1/1	0.76	0.14	72,72,72,72	0
58	MG	2A	3093	1/1	0.76	0.20	43,43,43,43	0
58	MG	1A	3304	1/1	0.76	0.21	43,43,43,43	0
58	MG	1A	3341	1/1	0.76	0.28	39,39,39,39	0
58	MG	2A	3750	1/1	0.76	0.21	60,60,60,60	0
58	MG	2A	3357	1/1	0.76	0.13	54,54,54,54	0
58	MG	1A	3771	1/1	0.76	0.31	40,40,40,40	0
58	MG	2B	215	1/1	0.76	0.15	68,68,68,68	0
58	MG	2A	3313	1/1	0.76	0.32	50,50,50,50	0
58	MG	1a	1802	1/1	0.76	0.16	69,69,69,69	0
58	MG	2A	3632	1/1	0.76	0.13	39,39,39,39	0
58	MG	1A	3989	1/1	0.76	0.15	38,38,38,38	0
58	MG	1A	3325	1/1	0.76	0.28	50,50,50,50	0
58	MG	2a	1688	1/1	0.77	0.23	65,65,65,65	0
58	MG	1a	1789	1/1	0.77	0.11	59,59,59,59	0
58	MG	2A	3110	1/1	0.77	0.23	50,50,50,50	0
58	MG	1a	1637	1/1	0.77	0.17	55,55,55,55	0
58	MG	2A	3475	1/1	0.77	0.19	52,52,52,52	0
58	MG	2A	3751	1/1	0.77	0.13	56,56,56,56	0
58	MG	1A	3776	1/1	0.77	0.10	60,60,60,60	0
58	MG	1A	3457	1/1	0.77	0.23	49,49,49,49	0
58	MG	2Y	201	1/1	0.77	0.36	53,53,53,53	0
58	MG	1A	4015	1/1	0.77	0.16	71,71,71,71	0
58	MG	2A	3343	1/1	0.77	0.20	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	18	105	1/1	0.77	0.35	50,50,50,50	0
58	MG	1A	3952	1/1	0.77	0.12	52,52,52,52	0
58	MG	1A	3094	1/1	0.77	0.20	42,42,42,42	0
58	MG	1a	1720	1/1	0.77	0.18	66,66,66,66	0
58	MG	1A	3620	1/1	0.77	0.18	28,28,28,28	0
58	MG	1x	108	1/1	0.77	0.22	30,30,30,30	0
58	MG	2a	1750	1/1	0.77	0.21	83,83,83,83	0
58	MG	1a	1665	1/1	0.77	0.11	60,60,60,60	0
58	MG	2A	3265	1/1	0.77	0.13	54,54,54,54	0
58	MG	2a	1633	1/1	0.77	0.32	54,54,54,54	0
58	MG	2A	3266	1/1	0.77	0.12	67,67,67,67	0
58	MG	1a	1666	1/1	0.77	0.17	63,63,63,63	0
58	MG	2A	3383	1/1	0.77	0.28	58,58,58,58	0
58	MG	1a	1607	1/1	0.77	0.18	62,62,62,62	0
58	MG	1a	1670	1/1	0.77	0.35	62,62,62,62	0
58	MG	2a	1796	1/1	0.77	0.20	57,57,57,57	0
58	MG	2A	3007	1/1	0.77	0.15	47,47,47,47	0
58	MG	2A	3395	1/1	0.77	0.25	52,52,52,52	0
58	MG	1A	4027	1/1	0.77	0.07	47,47,47,47	0
58	MG	1a	1757	1/1	0.77	0.18	60,60,60,60	0
58	MG	1A	3089	1/1	0.77	0.25	40,40,40,40	0
58	MG	1A	3206	1/1	0.77	0.20	51,51,51,51	0
58	MG	2a	1819	1/1	0.77	0.16	56,56,56,56	0
58	MG	1E	308	1/1	0.77	0.15	28,28,28,28	0
58	MG	1A	3581	1/1	0.77	0.33	32,32,32,32	0
58	MG	1A	4038	1/1	0.77	0.11	48,48,48,48	0
58	MG	2A	3706	1/1	0.77	0.19	49,49,49,49	0
58	MG	1a	1627	1/1	0.77	0.28	52,52,52,52	0
58	MG	1a	1779	1/1	0.77	0.13	55,55,55,55	0
58	MG	1A	3167	1/1	0.77	0.25	45,45,45,45	0
58	MG	1A	3402	1/1	0.77	0.31	48,48,48,48	0
58	MG	1B	216	1/1	0.78	0.17	65,65,65,65	0
58	MG	2A	3258	1/1	0.78	0.22	61,61,61,61	0
58	MG	2A	3497	1/1	0.78	0.27	46,46,46,46	0
58	MG	2a	1726	1/1	0.78	0.15	57,57,57,57	0
58	MG	1A	3588	1/1	0.78	0.18	29,29,29,29	0
58	MG	1A	3506	1/1	0.78	0.22	49,49,49,49	0
58	MG	2a	1627	1/1	0.78	0.18	66,66,66,66	0
58	MG	2A	3710	1/1	0.78	0.14	40,40,40,40	0
58	MG	2A	3327	1/1	0.78	0.14	72,72,72,72	0
58	MG	1A	3874	1/1	0.78	0.23	41,41,41,41	0
58	MG	2A	3717	1/1	0.78	0.22	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3720	1/1	0.78	0.12	67,67,67,67	0
58	MG	2A	3833	1/1	0.78	0.13	52,52,52,52	0
58	MG	1A	3707	1/1	0.78	0.15	30,30,30,30	0
58	MG	2A	3577	1/1	0.78	0.28	73,73,73,73	0
58	MG	2A	3736	1/1	0.78	0.14	51,51,51,51	0
58	MG	1I	106	1/1	0.78	0.20	51,51,51,51	0
58	MG	2B	210	1/1	0.78	0.08	75,75,75,75	0
58	MG	2a	1784	1/1	0.78	0.22	67,67,67,67	0
58	MG	1A	3529	1/1	0.78	0.15	58,58,58,58	0
58	MG	1F	304	1/1	0.78	0.28	63,63,63,63	0
58	MG	2A	3419	1/1	0.78	0.11	55,55,55,55	0
58	MG	2A	3429	1/1	0.78	0.27	52,52,52,52	0
58	MG	1a	1755	1/1	0.78	0.12	42,42,42,42	0
58	MG	2A	3760	1/1	0.78	0.11	45,45,45,45	0
58	MG	2A	3195	1/1	0.78	0.40	60,60,60,60	0
58	MG	18	107	1/1	0.78	0.41	62,62,62,62	0
58	MG	2A	3622	1/1	0.78	0.10	56,56,56,56	0
58	MG	2A	3778	1/1	0.78	0.24	58,58,58,58	0
58	MG	2A	3244	1/1	0.78	0.25	60,60,60,60	0
58	MG	1a	1698	1/1	0.78	0.15	52,52,52,52	0
58	MG	1A	3817	1/1	0.78	0.19	59,59,59,59	0
58	MG	2A	3210	1/1	0.78	0.22	55,55,55,55	0
58	MG	2A	3378	1/1	0.78	0.19	55,55,55,55	0
58	MG	2v	101	1/1	0.78	0.16	58,58,58,58	0
58	MG	1Q	204	1/1	0.78	0.15	34,34,34,34	0
58	MG	28	102	1/1	0.78	0.17	61,61,61,61	0
58	MG	1A	3255	1/1	0.78	0.37	58,58,58,58	0
58	MG	2x	105	1/1	0.78	0.17	63,63,63,63	0
58	MG	2A	3274	1/1	0.79	0.28	62,62,62,62	0
58	MG	2a	1685	1/1	0.79	0.35	54,54,54,54	0
58	MG	1A	3124	1/1	0.79	0.32	40,40,40,40	0
58	MG	1A	3536	1/1	0.79	0.18	55,55,55,55	0
58	MG	1A	3408	1/1	0.79	0.24	56,56,56,56	0
58	MG	2A	3759	1/1	0.79	0.44	68,68,68,68	0
58	MG	1A	3816	1/1	0.79	0.17	41,41,41,41	0
58	MG	2A	3594	1/1	0.79	0.18	61,61,61,61	0
58	MG	1A	4007	1/1	0.79	0.19	33,33,33,33	0
58	MG	1A	3456	1/1	0.79	0.39	62,62,62,62	0
58	MG	1A	3639	1/1	0.79	0.15	55,55,55,55	0
58	MG	1A	3354	1/1	0.79	0.27	59,59,59,59	0
58	MG	2A	3405	1/1	0.79	0.19	51,51,51,51	0
58	MG	1A	3677	1/1	0.79	0.21	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3790	1/1	0.79	0.17	55,55,55,55	0
58	MG	1A	3287	1/1	0.79	0.18	53,53,53,53	0
58	MG	1A	3059	1/1	0.79	0.21	42,42,42,42	0
58	MG	2A	3414	1/1	0.79	0.25	64,64,64,64	0
58	MG	2a	1611	1/1	0.79	0.18	66,66,66,66	0
58	MG	2a	1617	1/1	0.79	0.17	60,60,60,60	0
58	MG	1A	3082	1/1	0.79	0.21	34,34,34,34	0
58	MG	2a	1622	1/1	0.79	0.20	59,59,59,59	0
58	MG	2A	3317	1/1	0.79	0.35	67,67,67,67	0
58	MG	1A	3714	1/1	0.79	0.14	50,50,50,50	0
58	MG	2A	3808	1/1	0.79	0.12	50,50,50,50	0
58	MG	1A	3718	1/1	0.79	0.16	65,65,65,65	0
58	MG	1A	3269	1/1	0.79	0.30	49,49,49,49	0
58	MG	2a	1776	1/1	0.79	0.26	67,67,67,67	0
58	MG	13	104	1/1	0.79	0.27	48,48,48,48	0
58	MG	1A	4058	1/1	0.79	0.13	48,48,48,48	0
58	MG	2A	3249	1/1	0.79	0.24	64,64,64,64	0
58	MG	2A	3695	1/1	0.79	0.25	63,63,63,63	0
58	MG	1A	3493	1/1	0.79	0.23	43,43,43,43	0
58	MG	2A	3465	1/1	0.79	0.17	59,59,59,59	0
58	MG	2a	1642	1/1	0.79	0.18	62,62,62,62	0
58	MG	1A	3431	1/1	0.79	0.19	38,38,38,38	0
58	MG	2a	1647	1/1	0.79	0.13	69,69,69,69	0
58	MG	1A	3104	1/1	0.79	0.25	32,32,32,32	0
58	MG	2a	1813	1/1	0.79	0.19	54,54,54,54	0
58	MG	2A	3839	1/1	0.79	0.14	66,66,66,66	0
58	MG	1A	3590	1/1	0.79	0.16	48,48,48,48	0
58	MG	1A	3438	1/1	0.79	0.14	51,51,51,51	0
58	MG	1A	3601	1/1	0.79	0.50	56,56,56,56	0
58	MG	2A	3262	1/1	0.79	0.25	60,60,60,60	0
58	MG	2a	1655	1/1	0.79	0.16	56,56,56,56	0
58	MG	1B	213	1/1	0.79	0.26	57,57,57,57	0
58	MG	2A	3196	1/1	0.79	0.21	65,65,65,65	0
58	MG	2B	218	1/1	0.79	0.15	70,70,70,70	0
58	MG	1a	1771	1/1	0.79	0.07	45,45,45,45	0
58	MG	1A	3308	1/1	0.79	0.41	64,64,64,64	0
58	MG	1a	1761	1/1	0.80	0.12	68,68,68,68	0
58	MG	1A	3687	1/1	0.80	0.16	66,66,66,66	0
58	MG	2D	304	1/1	0.80	0.12	55,55,55,55	0
58	MG	1A	3465	1/1	0.80	0.40	66,66,66,66	0
58	MG	1A	3432	1/1	0.80	0.48	62,62,62,62	0
58	MG	2A	3214	1/1	0.80	0.30	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3996	1/1	0.80	0.21	47,47,47,47	0
58	MG	2A	3091	1/1	0.80	0.12	58,58,58,58	0
58	MG	2a	1706	1/1	0.80	0.21	63,63,63,63	0
58	MG	1A	3701	1/1	0.80	0.09	36,36,36,36	0
58	MG	2R	203	1/1	0.80	0.17	65,65,65,65	0
58	MG	1A	3866	1/1	0.80	0.21	52,52,52,52	0
58	MG	2A	3100	1/1	0.80	0.13	58,58,58,58	0
58	MG	1A	4011	1/1	0.80	0.12	44,44,44,44	0
58	MG	2A	3340	1/1	0.80	0.50	66,66,66,66	0
58	MG	1a	1689	1/1	0.80	0.30	55,55,55,55	0
58	MG	1A	3164	1/1	0.80	0.22	34,34,34,34	0
58	MG	2A	3125	1/1	0.80	0.26	45,45,45,45	0
58	MG	1A	4019	1/1	0.80	0.23	64,64,64,64	0
58	MG	1a	1624	1/1	0.80	0.09	50,50,50,50	0
58	MG	2A	3783	1/1	0.80	0.14	73,73,73,73	0
58	MG	2A	3134	1/1	0.80	0.25	57,57,57,57	0
58	MG	1a	1626	1/1	0.80	0.29	64,64,64,64	0
58	MG	2A	3366	1/1	0.80	0.24	67,67,67,67	0
58	MG	1A	3600	1/1	0.80	0.22	61,61,61,61	0
58	MG	1A	3886	1/1	0.80	0.10	45,45,45,45	0
58	MG	2A	3141	1/1	0.80	0.19	58,58,58,58	0
58	MG	1a	1633	1/1	0.80	0.14	58,58,58,58	0
58	MG	2A	3151	1/1	0.80	0.22	57,57,57,57	0
58	MG	1A	3539	1/1	0.80	0.42	50,50,50,50	0
58	MG	1A	3305	1/1	0.80	0.26	52,52,52,52	0
58	MG	1x	101	1/1	0.80	0.11	66,66,66,66	0
58	MG	1A	3039	1/1	0.80	0.54	35,35,35,35	0
58	MG	1A	3608	1/1	0.80	0.18	26,26,26,26	0
58	MG	1A	3416	1/1	0.80	0.16	49,49,49,49	0
58	MG	1A	3504	1/1	0.80	0.26	48,48,48,48	0
58	MG	1A	3069	1/1	0.80	0.31	61,61,61,61	0
58	MG	1a	1647	1/1	0.80	0.23	58,58,58,58	0
58	MG	2A	3409	1/1	0.80	0.23	62,62,62,62	0
58	MG	2a	1809	1/1	0.80	0.22	47,47,47,47	0
58	MG	2A	3827	1/1	0.80	0.12	41,41,41,41	0
58	MG	2A	3410	1/1	0.80	0.25	57,57,57,57	0
58	MG	2A	3179	1/1	0.80	0.46	62,62,62,62	0
58	MG	2A	3693	1/1	0.80	0.11	66,66,66,66	0
58	MG	1A	3407	1/1	0.80	0.19	37,37,37,37	0
58	MG	2B	204	1/1	0.80	0.14	72,72,72,72	0
58	MG	1A	3668	1/1	0.80	0.18	56,56,56,56	0
58	MG	2a	1654	1/1	0.80	0.23	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3285	1/1	0.80	0.21	43,43,43,43	0
58	MG	1A	3671	1/1	0.80	0.15	33,33,33,33	0
58	MG	2A	3201	1/1	0.80	0.12	67,67,67,67	0
58	MG	1a	1667	1/1	0.80	0.13	68,68,68,68	0
58	MG	2x	102	1/1	0.80	0.21	64,64,64,64	0
58	MG	1A	3462	1/1	0.80	0.27	62,62,62,62	0
58	MG	1A	3040	1/1	0.81	0.23	62,62,62,62	0
58	MG	1A	3074	1/1	0.81	0.26	59,59,59,59	0
58	MG	1n	101	1/1	0.81	0.18	57,57,57,57	0
58	MG	2A	3379	1/1	0.81	0.21	57,57,57,57	0
58	MG	2a	1659	1/1	0.81	0.31	71,71,71,71	0
58	MG	2a	1664	1/1	0.81	0.12	47,47,47,47	0
58	MG	1a	1709	1/1	0.81	0.15	56,56,56,56	0
58	MG	2A	3836	1/1	0.81	0.14	48,48,48,48	0
58	MG	1l	102	1/1	0.81	0.15	52,52,52,52	0
58	MG	2A	3146	1/1	0.81	0.21	52,52,52,52	0
58	MG	2A	3660	1/1	0.81	0.17	59,59,59,59	0
58	MG	1A	3135	1/1	0.81	0.16	53,53,53,53	0
58	MG	13	103	1/1	0.81	0.16	56,56,56,56	0
58	MG	2a	1686	1/1	0.81	0.16	56,56,56,56	0
58	MG	2A	3675	1/1	0.81	0.20	55,55,55,55	0
58	MG	1a	1729	1/1	0.81	0.15	55,55,55,55	0
58	MG	2A	3263	1/1	0.81	0.14	66,66,66,66	0
58	MG	2A	3264	1/1	0.81	0.12	54,54,54,54	0
58	MG	2a	1701	1/1	0.81	0.13	61,61,61,61	0
58	MG	1a	1652	1/1	0.81	0.13	61,61,61,61	0
58	MG	2a	1704	1/1	0.81	0.36	59,59,59,59	0
58	MG	1A	3251	1/1	0.81	0.26	59,59,59,59	0
58	MG	2A	3269	1/1	0.81	0.25	47,47,47,47	0
58	MG	2A	3408	1/1	0.81	0.22	56,56,56,56	0
58	MG	2a	1714	1/1	0.81	0.20	59,59,59,59	0
58	MG	1a	1661	1/1	0.81	0.09	58,58,58,58	0
58	MG	2A	3001	1/1	0.81	0.18	62,62,62,62	0
58	MG	1a	1662	1/1	0.81	0.29	55,55,55,55	0
58	MG	2a	1725	1/1	0.81	0.13	66,66,66,66	0
58	MG	1A	3478	1/1	0.81	0.21	37,37,37,37	0
58	MG	1A	3199	1/1	0.81	0.15	36,36,36,36	0
58	MG	2a	1735	1/1	0.81	0.12	57,57,57,57	0
58	MG	2F	303	1/1	0.81	0.20	58,58,58,58	0
58	MG	1A	3986	1/1	0.81	0.19	38,38,38,38	0
58	MG	2R	202	1/1	0.81	0.28	50,50,50,50	0
58	MG	2A	3721	1/1	0.81	0.17	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1B	211	1/1	0.81	0.14	50,50,50,50	0
58	MG	2A	3432	1/1	0.81	0.13	70,70,70,70	0
58	MG	2A	3435	1/1	0.81	0.24	55,55,55,55	0
58	MG	2A	3186	1/1	0.81	0.37	58,58,58,58	0
58	MG	2A	3440	1/1	0.81	0.17	52,52,52,52	0
58	MG	2A	3290	1/1	0.81	0.17	47,47,47,47	0
58	MG	2A	3189	1/1	0.81	0.34	64,64,64,64	0
58	MG	2A	3193	1/1	0.81	0.31	64,64,64,64	0
58	MG	2a	1774	1/1	0.81	0.16	49,49,49,49	0
58	MG	1A	3309	1/1	0.81	0.24	57,57,57,57	0
58	MG	1A	3543	1/1	0.81	0.18	54,54,54,54	0
58	MG	1A	3547	1/1	0.81	0.22	57,57,57,57	0
58	MG	2a	1790	1/1	0.81	0.13	60,60,60,60	0
58	MG	1A	3728	1/1	0.81	0.27	70,70,70,70	0
58	MG	2A	3053	1/1	0.81	0.17	63,63,63,63	0
58	MG	2A	3055	1/1	0.81	0.31	68,68,68,68	0
58	MG	1A	3314	1/1	0.81	0.21	52,52,52,52	0
58	MG	2A	3081	1/1	0.81	0.18	50,50,50,50	0
58	MG	1A	3912	1/1	0.81	0.15	39,39,39,39	0
58	MG	1A	3034	1/1	0.81	0.16	32,32,32,32	0
58	MG	1A	3927	1/1	0.81	0.08	44,44,44,44	0
58	MG	1A	3560	1/1	0.81	0.24	63,63,63,63	0
58	MG	1a	1782	1/1	0.81	0.14	51,51,51,51	0
58	MG	2A	3103	1/1	0.81	0.17	56,56,56,56	0
58	MG	2A	3798	1/1	0.81	0.18	47,47,47,47	0
58	MG	1A	3062	1/1	0.81	0.11	41,41,41,41	0
58	MG	1A	3450	1/1	0.81	0.27	65,65,65,65	0
58	MG	2A	3115	1/1	0.81	0.23	69,69,69,69	0
58	MG	1Q	206	1/1	0.81	0.20	58,58,58,58	0
58	MG	1A	3770	1/1	0.81	0.14	30,30,30,30	0
58	MG	2a	1644	1/1	0.81	0.17	67,67,67,67	0
58	MG	1A	3950	1/1	0.81	0.14	57,57,57,57	0
58	MG	2A	3608	1/1	0.81	0.18	34,34,34,34	0
58	MG	1A	3374	1/1	0.81	0.24	40,40,40,40	0
58	MG	2A	3243	1/1	0.81	0.39	62,62,62,62	0
58	MG	1A	3415	1/1	0.81	0.15	69,69,69,69	0
60	ZN	2n	102	1/1	0.81	0.05	86,86,86,86	0
58	MG	2Q	203	1/1	0.82	0.22	62,62,62,62	0
58	MG	1A	3088	1/1	0.82	0.18	32,32,32,32	0
58	MG	2A	3762	1/1	0.82	0.15	66,66,66,66	0
58	MG	1A	3002	1/1	0.82	0.35	55,55,55,55	0
58	MG	2T	201	1/1	0.82	0.18	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3943	1/1	0.82	0.08	38,38,38,38	0
58	MG	2A	3292	1/1	0.82	0.14	57,57,57,57	0
58	MG	2A	3229	1/1	0.82	0.27	41,41,41,41	0
58	MG	2A	3017	1/1	0.82	0.28	38,38,38,38	0
58	MG	2A	3598	1/1	0.82	0.26	50,50,50,50	0
58	MG	2A	3602	1/1	0.82	0.08	57,57,57,57	0
58	MG	28	104	1/1	0.82	0.18	55,55,55,55	0
58	MG	1A	4009	1/1	0.82	0.08	40,40,40,40	0
58	MG	1A	3705	1/1	0.82	0.31	66,66,66,66	0
58	MG	1a	1638	1/1	0.82	0.16	62,62,62,62	0
58	MG	1A	3362	1/1	0.82	0.15	61,61,61,61	0
58	MG	12	101	1/1	0.82	0.27	50,50,50,50	0
58	MG	2a	1615	1/1	0.82	0.09	57,57,57,57	0
58	MG	1A	3109	1/1	0.82	0.21	33,33,33,33	0
58	MG	1A	3183	1/1	0.82	0.19	39,39,39,39	0
58	MG	2a	1620	1/1	0.82	0.19	74,74,74,74	0
58	MG	17	105	1/1	0.82	0.21	52,52,52,52	0
58	MG	2A	3056	1/1	0.82	0.29	60,60,60,60	0
58	MG	1a	1788	1/1	0.82	0.19	76,76,76,76	0
58	MG	18	103	1/1	0.82	0.22	35,35,35,35	0
58	MG	2A	3329	1/1	0.82	0.51	59,59,59,59	0
58	MG	1A	3213	1/1	0.82	0.11	58,58,58,58	0
58	MG	1A	3121	1/1	0.82	0.26	39,39,39,39	0
58	MG	1A	3848	1/1	0.82	0.10	61,61,61,61	0
58	MG	2a	1760	1/1	0.82	0.08	74,74,74,74	0
58	MG	2A	3442	1/1	0.82	0.35	55,55,55,55	0
58	MG	1D	303	1/1	0.82	0.16	58,58,58,58	0
58	MG	1A	3644	1/1	0.82	0.14	36,36,36,36	0
58	MG	1A	3399	1/1	0.82	0.25	46,46,46,46	0
58	MG	2A	3346	1/1	0.82	0.14	63,63,63,63	0
58	MG	1a	1735	1/1	0.82	0.24	61,61,61,61	0
58	MG	1A	4032	1/1	0.82	0.10	38,38,38,38	0
58	MG	2A	3466	1/1	0.82	0.21	59,59,59,59	0
58	MG	2a	1799	1/1	0.82	0.26	62,62,62,62	0
58	MG	2A	3709	1/1	0.82	0.27	55,55,55,55	0
58	MG	1F	309	1/1	0.82	0.17	37,37,37,37	0
58	MG	1A	3494	1/1	0.82	0.25	57,57,57,57	0
58	MG	1A	3268	1/1	0.82	0.22	60,60,60,60	0
58	MG	2A	3364	1/1	0.82	0.16	59,59,59,59	0
58	MG	1a	1749	1/1	0.82	0.14	50,50,50,50	0
58	MG	1A	3594	1/1	0.82	0.34	59,59,59,59	0
58	MG	2A	3726	1/1	0.82	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	2A	3495	1/1	0.82	0.07	64,64,64,64	0
58	MG	2a	1662	1/1	0.82	0.27	54,54,54,54	0
58	MG	2A	3275	1/1	0.82	0.15	62,62,62,62	0
58	MG	2A	3502	1/1	0.82	0.12	53,53,53,53	0
58	MG	1Q	207	1/1	0.82	0.25	58,58,58,58	0
58	MG	2a	1674	1/1	0.82	0.20	68,68,68,68	0
58	MG	2A	3525	1/1	0.82	0.18	37,37,37,37	0
58	MG	2A	3532	1/1	0.82	0.15	52,52,52,52	0
58	MG	1A	3545	1/1	0.82	0.34	54,54,54,54	0
58	MG	1A	3353	1/1	0.82	0.23	56,56,56,56	0
58	MG	2A	3283	1/1	0.82	0.14	62,62,62,62	0
58	MG	2A	3563	1/1	0.82	0.14	44,44,44,44	0
58	MG	2Q	202	1/1	0.82	0.12	58,58,58,58	0
58	MG	1A	3894	1/1	0.83	0.10	42,42,42,42	0
58	MG	2A	3377	1/1	0.83	0.10	70,70,70,70	0
58	MG	1a	1777	1/1	0.83	0.13	50,50,50,50	0
58	MG	2A	3060	1/1	0.83	0.17	62,62,62,62	0
58	MG	2A	3064	1/1	0.83	0.18	63,63,63,63	0
58	MG	1A	3911	1/1	0.83	0.15	49,49,49,49	0
58	MG	2A	3199	1/1	0.83	0.21	47,47,47,47	0
58	MG	2A	3779	1/1	0.83	0.13	54,54,54,54	0
58	MG	2a	1708	1/1	0.83	0.14	60,60,60,60	0
58	MG	23	101	1/1	0.83	0.16	63,63,63,63	0
58	MG	1A	3242	1/1	0.83	0.20	48,48,48,48	0
58	MG	2a	1713	1/1	0.83	0.15	43,43,43,43	0
58	MG	1A	3068	1/1	0.83	0.18	27,27,27,27	0
58	MG	2A	3786	1/1	0.83	0.17	70,70,70,70	0
58	MG	1O	205	1/1	0.83	0.13	54,54,54,54	0
58	MG	2A	3092	1/1	0.83	0.08	70,70,70,70	0
58	MG	1A	3516	1/1	0.83	0.24	44,44,44,44	0
58	MG	2A	3603	1/1	0.83	0.20	67,67,67,67	0
58	MG	1A	3665	1/1	0.83	0.20	24,24,24,24	0
58	MG	1A	3035	1/1	0.83	0.43	44,44,44,44	0
58	MG	1A	3385	1/1	0.83	0.27	68,68,68,68	0
58	MG	1S	203	1/1	0.83	0.20	62,62,62,62	0
58	MG	1A	3130	1/1	0.83	0.17	57,57,57,57	0
58	MG	1A	3674	1/1	0.83	0.22	32,32,32,32	0
58	MG	2A	3310	1/1	0.83	0.13	60,60,60,60	0
58	MG	1A	3395	1/1	0.83	0.26	51,51,51,51	0
58	MG	1b	301	1/1	0.83	0.11	75,75,75,75	0
58	MG	1A	3786	1/1	0.83	0.18	48,48,48,48	0
58	MG	2A	3423	1/1	0.83	0.22	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3425	1/1	0.83	0.16	47,47,47,47	0
58	MG	1A	3953	1/1	0.83	0.21	48,48,48,48	0
58	MG	1a	1728	1/1	0.83	0.08	64,64,64,64	0
58	MG	1A	3428	1/1	0.83	0.15	45,45,45,45	0
58	MG	2a	1764	1/1	0.83	0.09	74,74,74,74	0
58	MG	2a	1768	1/1	0.83	0.08	69,69,69,69	0
58	MG	2a	1639	1/1	0.83	0.18	67,67,67,67	0
58	MG	1A	3473	1/1	0.83	0.18	51,51,51,51	0
58	MG	1A	3131	1/1	0.83	0.24	44,44,44,44	0
58	MG	12	102	1/1	0.83	0.26	34,34,34,34	0
58	MG	2A	3330	1/1	0.83	0.25	59,59,59,59	0
58	MG	1A	3960	1/1	0.83	0.12	40,40,40,40	0
58	MG	1A	3961	1/1	0.83	0.12	41,41,41,41	0
58	MG	1A	3595	1/1	0.83	0.24	63,63,63,63	0
58	MG	2A	3337	1/1	0.83	0.35	57,57,57,57	0
58	MG	1A	4088	1/1	0.83	0.15	67,67,67,67	0
58	MG	2A	3342	1/1	0.83	0.10	63,63,63,63	0
58	MG	2B	214	1/1	0.83	0.13	56,56,56,56	0
58	MG	1A	3179	1/1	0.83	0.20	53,53,53,53	0
58	MG	1A	3055	1/1	0.83	0.14	43,43,43,43	0
58	MG	1A	3852	1/1	0.83	0.18	46,46,46,46	0
58	MG	2a	1658	1/1	0.83	0.09	70,70,70,70	0
58	MG	1A	3854	1/1	0.83	0.13	51,51,51,51	0
58	MG	2a	1661	1/1	0.83	0.28	65,65,65,65	0
58	MG	2A	3027	1/1	0.83	0.30	58,58,58,58	0
58	MG	1A	3295	1/1	0.83	0.12	67,67,67,67	0
58	MG	1a	1675	1/1	0.83	0.19	44,44,44,44	0
58	MG	2a	1670	1/1	0.83	0.12	56,56,56,56	0
58	MG	1A	3436	1/1	0.83	0.27	56,56,56,56	0
58	MG	2A	3501	1/1	0.83	0.14	59,59,59,59	0
58	MG	1A	3358	1/1	0.83	0.18	43,43,43,43	0
58	MG	2A	3506	1/1	0.83	0.13	55,55,55,55	0
58	MG	1A	3237	1/1	0.83	0.28	39,39,39,39	0
58	MG	1A	3558	1/1	0.83	0.30	33,33,33,33	0
58	MG	2A	3373	1/1	0.83	0.11	49,49,49,49	0
58	MG	2A	3534	1/1	0.83	0.20	50,50,50,50	0
58	MG	1A	3999	1/1	0.84	0.20	26,26,26,26	0
58	MG	2A	3576	1/1	0.84	0.07	52,52,52,52	0
58	MG	2A	3002	1/1	0.84	0.17	63,63,63,63	0
58	MG	2A	3367	1/1	0.84	0.23	54,54,54,54	0
58	MG	1a	1656	1/1	0.84	0.16	64,64,64,64	0
58	MG	2A	3371	1/1	0.84	0.09	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2a	1663	1/1	0.84	0.28	53,53,53,53	0
58	MG	1A	4090	1/1	0.84	0.27	59,59,59,59	0
58	MG	2A	3260	1/1	0.84	0.32	58,58,58,58	0
58	MG	2A	3376	1/1	0.84	0.30	57,57,57,57	0
58	MG	1B	205	1/1	0.84	0.14	49,49,49,49	0
58	MG	2a	1673	1/1	0.84	0.09	57,57,57,57	0
58	MG	2A	3604	1/1	0.84	0.12	41,41,41,41	0
58	MG	1B	206	1/1	0.84	0.31	47,47,47,47	0
58	MG	1a	1751	1/1	0.84	0.14	45,45,45,45	0
58	MG	2A	3171	1/1	0.84	0.26	54,54,54,54	0
58	MG	2A	3172	1/1	0.84	0.27	47,47,47,47	0
58	MG	14	101	1/1	0.84	0.15	64,64,64,64	0
58	MG	15	102	1/1	0.84	0.20	44,44,44,44	0
58	MG	2B	206	1/1	0.84	0.25	64,64,64,64	0
58	MG	2A	3176	1/1	0.84	0.20	64,64,64,64	0
58	MG	2A	3178	1/1	0.84	0.55	60,60,60,60	0
58	MG	1B	209	1/1	0.84	0.20	46,46,46,46	0
58	MG	2A	3278	1/1	0.84	0.15	66,66,66,66	0
58	MG	2A	3641	1/1	0.84	0.12	57,57,57,57	0
58	MG	1A	3930	1/1	0.84	0.16	41,41,41,41	0
58	MG	2A	3652	1/1	0.84	0.15	49,49,49,49	0
58	MG	2A	3183	1/1	0.84	0.16	66,66,66,66	0
58	MG	1A	3296	1/1	0.84	0.10	41,41,41,41	0
58	MG	2A	3047	1/1	0.84	0.21	66,66,66,66	0
58	MG	1A	3212	1/1	0.84	0.15	42,42,42,42	0
58	MG	1A	3489	1/1	0.84	0.27	45,45,45,45	0
58	MG	1A	3370	1/1	0.84	0.24	49,49,49,49	0
58	MG	2A	3688	1/1	0.84	0.10	59,59,59,59	0
58	MG	2A	3291	1/1	0.84	0.20	61,61,61,61	0
58	MG	1a	1605	1/1	0.84	0.12	50,50,50,50	0
58	MG	1A	3711	1/1	0.84	0.16	35,35,35,35	0
58	MG	1a	1680	1/1	0.84	0.23	65,65,65,65	0
58	MG	1A	3672	1/1	0.84	0.17	34,34,34,34	0
58	MG	2A	3301	1/1	0.84	0.56	63,63,63,63	0
58	MG	2A	3204	1/1	0.84	0.31	49,49,49,49	0
58	MG	1A	3717	1/1	0.84	0.17	54,54,54,54	0
58	MG	2A	3436	1/1	0.84	0.19	43,43,43,43	0
58	MG	2a	1745	1/1	0.84	0.13	70,70,70,70	0
58	MG	2U	201	1/1	0.84	0.27	44,44,44,44	0
58	MG	1A	4023	1/1	0.84	0.13	52,52,52,52	0
58	MG	2A	3311	1/1	0.84	0.20	59,59,59,59	0
58	MG	1A	4024	1/1	0.84	0.12	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	3445	1/1	0.84	0.10	58,58,58,58	0
58	MG	2a	1754	1/1	0.84	0.22	59,59,59,59	0
58	MG	2A	3314	1/1	0.84	0.50	70,70,70,70	0
58	MG	1A	3523	1/1	0.84	0.13	68,68,68,68	0
58	MG	1A	3885	1/1	0.84	0.17	38,38,38,38	0
58	MG	1A	3781	1/1	0.84	0.15	45,45,45,45	0
58	MG	2A	3742	1/1	0.84	0.18	38,38,38,38	0
58	MG	2a	1765	1/1	0.84	0.20	60,60,60,60	0
58	MG	1A	3675	1/1	0.84	0.13	39,39,39,39	0
58	MG	1A	3888	1/1	0.84	0.22	43,43,43,43	0
58	MG	1A	4034	1/1	0.84	0.25	42,42,42,42	0
58	MG	1A	3890	1/1	0.84	0.21	33,33,33,33	0
58	MG	2a	1616	1/1	0.84	0.23	58,58,58,58	0
58	MG	1A	3893	1/1	0.84	0.17	47,47,47,47	0
58	MG	2A	3232	1/1	0.84	0.43	47,47,47,47	0
58	MG	1A	4041	1/1	0.84	0.34	41,41,41,41	0
58	MG	1A	3791	1/1	0.84	0.07	52,52,52,52	0
58	MG	1A	3897	1/1	0.84	0.16	25,25,25,25	0
58	MG	2a	1801	1/1	0.84	0.21	59,59,59,59	0
58	MG	2A	3768	1/1	0.84	0.13	63,63,63,63	0
58	MG	2A	3490	1/1	0.84	0.12	56,56,56,56	0
58	MG	2A	3491	1/1	0.84	0.24	59,59,59,59	0
58	MG	1n	102	1/1	0.84	0.13	43,43,43,43	0
58	MG	2A	3239	1/1	0.84	0.14	68,68,68,68	0
58	MG	2A	3240	1/1	0.84	0.24	67,67,67,67	0
58	MG	1a	1713	1/1	0.84	0.12	71,71,71,71	0
58	MG	2A	3504	1/1	0.84	0.19	35,35,35,35	0
58	MG	1A	3977	1/1	0.84	0.18	43,43,43,43	0
58	MG	2A	3514	1/1	0.84	0.33	54,54,54,54	0
58	MG	1A	3391	1/1	0.84	0.18	38,38,38,38	0
58	MG	2k	201	1/1	0.84	0.16	58,58,58,58	0
58	MG	2A	3348	1/1	0.84	0.19	57,57,57,57	0
58	MG	2A	3531	1/1	0.84	0.24	65,65,65,65	0
58	MG	1A	3804	1/1	0.84	0.15	44,44,44,44	0
58	MG	2A	3350	1/1	0.84	0.17	68,68,68,68	0
58	MG	1l	101	1/1	0.84	0.25	40,40,40,40	0
58	MG	1A	3544	1/1	0.84	0.33	64,64,64,64	0
58	MG	1A	3463	1/1	0.84	0.15	63,63,63,63	0
58	MG	2A	3804	1/1	0.84	0.10	49,49,49,49	0
58	MG	2A	3805	1/1	0.84	0.16	40,40,40,40	0
58	MG	1a	1740	1/1	0.84	0.15	40,40,40,40	0
58	MG	1a	1673	1/1	0.85	0.15	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1a	1603	1/1	0.85	0.18	53,53,53,53	0
58	MG	2A	3834	1/1	0.85	0.10	57,57,57,57	0
58	MG	2A	3298	1/1	0.85	0.30	62,62,62,62	0
58	MG	1a	1765	1/1	0.85	0.14	45,45,45,45	0
58	MG	1A	3896	1/1	0.85	0.11	30,30,30,30	0
58	MG	2A	3306	1/1	0.85	0.10	43,43,43,43	0
58	MG	1A	3963	1/1	0.85	0.16	30,30,30,30	0
58	MG	1E	310	1/1	0.85	0.16	62,62,62,62	0
58	MG	2A	3062	1/1	0.85	0.27	59,59,59,59	0
58	MG	2a	1679	1/1	0.85	0.12	54,54,54,54	0
58	MG	2a	1680	1/1	0.85	0.11	58,58,58,58	0
58	MG	2A	3063	1/1	0.85	0.21	60,60,60,60	0
58	MG	1E	312	1/1	0.85	0.24	50,50,50,50	0
58	MG	2B	211	1/1	0.85	0.09	69,69,69,69	0
58	MG	1A	4033	1/1	0.85	0.07	41,41,41,41	0
58	MG	2A	3677	1/1	0.85	0.14	68,68,68,68	0
58	MG	1A	3149	1/1	0.85	0.19	32,32,32,32	0
58	MG	1a	1778	1/1	0.85	0.05	62,62,62,62	0
58	MG	2A	3320	1/1	0.85	0.27	57,57,57,57	0
58	MG	2A	3088	1/1	0.85	0.29	48,48,48,48	0
58	MG	1A	3441	1/1	0.85	0.23	44,44,44,44	0
58	MG	2A	3450	1/1	0.85	0.14	58,58,58,58	0
58	MG	2A	3699	1/1	0.85	0.17	57,57,57,57	0
58	MG	1A	3635	1/1	0.85	0.10	47,47,47,47	0
58	MG	1a	1783	1/1	0.85	0.10	47,47,47,47	0
58	MG	2E	308	1/1	0.85	0.23	50,50,50,50	0
58	MG	1A	3978	1/1	0.85	0.09	65,65,65,65	0
58	MG	2A	3328	1/1	0.85	0.10	68,68,68,68	0
58	MG	2N	201	1/1	0.85	0.26	51,51,51,51	0
58	MG	2a	1720	1/1	0.85	0.20	60,60,60,60	0
58	MG	2A	3228	1/1	0.85	0.21	52,52,52,52	0
58	MG	1A	3982	1/1	0.85	0.07	55,55,55,55	0
58	MG	1A	3696	1/1	0.85	0.17	27,27,27,27	0
58	MG	1A	3926	1/1	0.85	0.12	35,35,35,35	0
58	MG	1A	3841	1/1	0.85	0.16	51,51,51,51	0
58	MG	2A	3723	1/1	0.85	0.10	53,53,53,53	0
58	MG	2a	1736	1/1	0.85	0.34	62,62,62,62	0
58	MG	2A	3480	1/1	0.85	0.13	45,45,45,45	0
58	MG	1U	202	1/1	0.85	0.36	46,46,46,46	0
58	MG	1A	3843	1/1	0.85	0.22	58,58,58,58	0
58	MG	2A	3123	1/1	0.85	0.21	59,59,59,59	0
58	MG	1a	1801	1/1	0.85	0.36	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	3493	1/1	0.85	0.19	61,61,61,61	0
58	MG	1A	3937	1/1	0.85	0.19	32,32,32,32	0
58	MG	2A	3496	1/1	0.85	0.24	60,60,60,60	0
58	MG	1A	3050	1/1	0.85	0.26	40,40,40,40	0
58	MG	1a	1805	1/1	0.85	0.11	58,58,58,58	0
58	MG	1a	1711	1/1	0.85	0.20	50,50,50,50	0
58	MG	1A	3163	1/1	0.85	0.12	47,47,47,47	0
58	MG	1e	201	1/1	0.85	0.16	63,63,63,63	0
58	MG	2A	3761	1/1	0.85	0.13	44,44,44,44	0
58	MG	1A	3765	1/1	0.85	0.22	36,36,36,36	0
58	MG	2A	3518	1/1	0.85	0.22	51,51,51,51	0
58	MG	2A	3143	1/1	0.85	0.15	51,51,51,51	0
58	MG	1a	1715	1/1	0.85	0.18	34,34,34,34	0
58	MG	1A	4097	1/1	0.85	0.12	41,41,41,41	0
58	MG	2A	3147	1/1	0.85	0.21	54,54,54,54	0
58	MG	1A	4099	1/1	0.85	0.26	50,50,50,50	0
58	MG	2a	1779	1/1	0.85	0.33	59,59,59,59	0
58	MG	2A	3154	1/1	0.85	0.09	54,54,54,54	0
58	MG	2a	1625	1/1	0.85	0.16	61,61,61,61	0
58	MG	1a	1727	1/1	0.85	0.12	52,52,52,52	0
58	MG	2A	3551	1/1	0.85	0.13	65,65,65,65	0
58	MG	2a	1795	1/1	0.85	0.16	64,64,64,64	0
58	MG	2A	3556	1/1	0.85	0.21	31,31,31,31	0
58	MG	2A	3558	1/1	0.85	0.21	59,59,59,59	0
58	MG	1A	4102	1/1	0.85	0.28	55,55,55,55	0
58	MG	2A	3791	1/1	0.85	0.27	52,52,52,52	0
58	MG	1B	201	1/1	0.85	0.21	45,45,45,45	0
58	MG	1A	3316	1/1	0.85	0.17	35,35,35,35	0
58	MG	2A	3797	1/1	0.85	0.13	47,47,47,47	0
58	MG	1A	3480	1/1	0.85	0.19	36,36,36,36	0
58	MG	1A	4017	1/1	0.85	0.19	46,46,46,46	0
58	MG	1a	1660	1/1	0.85	0.21	52,52,52,52	0
58	MG	1A	3405	1/1	0.85	0.19	41,41,41,41	0
58	MG	1A	3774	1/1	0.85	0.23	30,30,30,30	0
58	MG	1a	1745	1/1	0.85	0.10	52,52,52,52	0
58	MG	1A	3323	1/1	0.85	0.22	38,38,38,38	0
58	MG	1A	3716	1/1	0.85	0.22	51,51,51,51	0
58	MG	1A	3607	1/1	0.85	0.24	46,46,46,46	0
58	MG	2A	3022	1/1	0.85	0.32	50,50,50,50	0
58	MG	1A	3260	1/1	0.85	0.31	51,51,51,51	0
58	MG	1A	3524	1/1	0.85	0.21	47,47,47,47	0
58	MG	2A	3821	1/1	0.85	0.22	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	3184	1/1	0.85	0.15	73,73,73,73	0
58	MG	1a	1756	1/1	0.85	0.12	45,45,45,45	0
58	MG	1A	3676	1/1	0.85	0.12	43,43,43,43	0
58	MG	2x	104	1/1	0.85	0.15	64,64,64,64	0
58	MG	2a	1660	1/1	0.85	0.13	65,65,65,65	0
58	MG	1a	1602	1/1	0.85	0.19	64,64,64,64	0
58	MG	2A	3819	1/1	0.86	0.08	56,56,56,56	0
58	MG	2A	3611	1/1	0.86	0.06	53,53,53,53	0
58	MG	2A	3417	1/1	0.86	0.26	52,52,52,52	0
58	MG	1A	3004	1/1	0.86	0.27	36,36,36,36	0
58	MG	1B	214	1/1	0.86	0.15	61,61,61,61	0
58	MG	1B	215	1/1	0.86	0.15	63,63,63,63	0
58	MG	2A	3308	1/1	0.86	0.25	45,45,45,45	0
58	MG	2A	3427	1/1	0.86	0.26	43,43,43,43	0
58	MG	2A	3070	1/1	0.86	0.17	55,55,55,55	0
58	MG	1A	3939	1/1	0.86	0.21	52,52,52,52	0
58	MG	2A	3644	1/1	0.86	0.23	63,63,63,63	0
58	MG	1B	222	1/1	0.86	0.23	37,37,37,37	0
58	MG	2A	3650	1/1	0.86	0.26	61,61,61,61	0
58	MG	1A	3360	1/1	0.86	0.25	52,52,52,52	0
58	MG	2A	3657	1/1	0.86	0.13	61,61,61,61	0
58	MG	1A	3472	1/1	0.86	0.38	51,51,51,51	0
58	MG	2A	3661	1/1	0.86	0.27	55,55,55,55	0
58	MG	1A	3246	1/1	0.86	0.23	48,48,48,48	0
58	MG	1a	1611	1/1	0.86	0.09	52,52,52,52	0
58	MG	2A	3671	1/1	0.86	0.17	58,58,58,58	0
58	MG	2a	1691	1/1	0.86	0.23	50,50,50,50	0
58	MG	1A	3327	1/1	0.86	0.29	45,45,45,45	0
58	MG	1A	3301	1/1	0.86	0.22	43,43,43,43	0
58	MG	2B	217	1/1	0.86	0.12	52,52,52,52	0
58	MG	2A	3099	1/1	0.86	0.19	60,60,60,60	0
58	MG	1A	3116	1/1	0.86	0.18	29,29,29,29	0
58	MG	1a	1796	1/1	0.86	0.08	39,39,39,39	0
58	MG	1A	3019	1/1	0.86	0.20	34,34,34,34	0
58	MG	2A	3461	1/1	0.86	0.20	38,38,38,38	0
58	MG	2A	3462	1/1	0.86	0.27	53,53,53,53	0
58	MG	1a	1799	1/1	0.86	0.18	46,46,46,46	0
58	MG	1a	1800	1/1	0.86	0.21	68,68,68,68	0
58	MG	1A	3738	1/1	0.86	0.18	77,77,77,77	0
58	MG	1A	3864	1/1	0.86	0.13	43,43,43,43	0
58	MG	2F	302	1/1	0.86	0.20	44,44,44,44	0
58	MG	2A	3470	1/1	0.86	0.13	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	2F	306	1/1	0.86	0.23	59,59,59,59	0
58	MG	1A	3054	1/1	0.86	0.10	45,45,45,45	0
58	MG	2A	3334	1/1	0.86	0.30	67,67,67,67	0
58	MG	1N	201	1/1	0.86	0.35	47,47,47,47	0
58	MG	2A	3716	1/1	0.86	0.16	38,38,38,38	0
58	MG	1a	1807	1/1	0.86	0.23	56,56,56,56	0
58	MG	1A	3445	1/1	0.86	0.32	36,36,36,36	0
58	MG	2A	3482	1/1	0.86	0.30	56,56,56,56	0
58	MG	1A	3181	1/1	0.86	0.16	54,54,54,54	0
58	MG	2a	1743	1/1	0.86	0.13	56,56,56,56	0
58	MG	1a	1629	1/1	0.86	0.15	55,55,55,55	0
58	MG	1a	1631	1/1	0.86	0.30	57,57,57,57	0
58	MG	1A	3744	1/1	0.86	0.13	47,47,47,47	0
58	MG	1A	3598	1/1	0.86	0.31	48,48,48,48	0
58	MG	2A	3740	1/1	0.86	0.33	47,47,47,47	0
58	MG	1w	107	1/1	0.86	0.11	35,35,35,35	0
58	MG	1A	4042	1/1	0.86	0.22	28,28,28,28	0
58	MG	2A	3746	1/1	0.86	0.13	59,59,59,59	0
58	MG	2A	3499	1/1	0.86	0.18	66,66,66,66	0
58	MG	1A	3599	1/1	0.86	0.17	32,32,32,32	0
58	MG	2A	3150	1/1	0.86	0.07	52,52,52,52	0
58	MG	2a	1603	1/1	0.86	0.24	58,58,58,58	0
58	MG	2a	1762	1/1	0.86	0.13	67,67,67,67	0
58	MG	1A	4053	1/1	0.86	0.15	54,54,54,54	0
58	MG	1x	106	1/1	0.86	0.19	54,54,54,54	0
58	MG	2a	1609	1/1	0.86	0.12	64,64,64,64	0
58	MG	2A	3511	1/1	0.86	0.17	35,35,35,35	0
58	MG	2a	1614	1/1	0.86	0.15	58,58,58,58	0
58	MG	1A	3310	1/1	0.86	0.17	45,45,45,45	0
58	MG	1V	206	1/1	0.86	0.16	43,43,43,43	0
58	MG	1a	1736	1/1	0.86	0.15	48,48,48,48	0
58	MG	2a	1786	1/1	0.86	0.14	67,67,67,67	0
58	MG	2A	3524	1/1	0.86	0.20	61,61,61,61	0
58	MG	1A	3974	1/1	0.86	0.08	72,72,72,72	0
58	MG	2a	1621	1/1	0.86	0.17	70,70,70,70	0
58	MG	2A	3370	1/1	0.86	0.29	57,57,57,57	0
58	MG	1A	3684	1/1	0.86	0.16	53,53,53,53	0
58	MG	2A	3167	1/1	0.86	0.25	37,37,37,37	0
58	MG	2A	3268	1/1	0.86	0.37	51,51,51,51	0
58	MG	2A	3781	1/1	0.86	0.25	51,51,51,51	0
58	MG	1a	1646	1/1	0.86	0.14	42,42,42,42	0
58	MG	1A	3126	1/1	0.86	0.15	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3554	1/1	0.86	0.22	44,44,44,44	0
58	MG	1a	1650	1/1	0.86	0.14	38,38,38,38	0
58	MG	1A	3689	1/1	0.86	0.14	40,40,40,40	0
58	MG	1A	3980	1/1	0.86	0.09	40,40,40,40	0
58	MG	1A	3602	1/1	0.86	0.34	55,55,55,55	0
58	MG	2A	3569	1/1	0.86	0.08	42,42,42,42	0
58	MG	1A	3495	1/1	0.86	0.22	56,56,56,56	0
58	MG	2d	301	1/1	0.86	0.22	51,51,51,51	0
58	MG	2A	3177	1/1	0.86	0.15	47,47,47,47	0
58	MG	1A	4096	1/1	0.86	0.14	40,40,40,40	0
58	MG	2A	3282	1/1	0.86	0.16	70,70,70,70	0
58	MG	1A	3497	1/1	0.86	0.23	27,27,27,27	0
58	MG	1A	3502	1/1	0.86	0.23	51,51,51,51	0
58	MG	1A	3919	1/1	0.86	0.20	34,34,34,34	0
58	MG	1A	3922	1/1	0.86	0.18	48,48,48,48	0
58	MG	1A	3703	1/1	0.86	0.26	29,29,29,29	0
58	MG	1A	3027	1/1	0.86	0.14	63,63,63,63	0
58	MG	16	101	1/1	0.86	0.22	56,56,56,56	0
58	MG	1A	3187	1/1	0.86	0.34	38,38,38,38	0
58	MG	1A	3929	1/1	0.86	0.17	32,32,32,32	0
60	ZN	24	501	1/1	0.86	0.07	103,103,103,103	0
58	MG	1A	3810	1/1	0.86	0.11	50,50,50,50	0
58	MG	2a	1692	1/1	0.87	0.19	60,60,60,60	0
58	MG	2a	1695	1/1	0.87	0.12	51,51,51,51	0
58	MG	2A	3769	1/1	0.87	0.10	36,36,36,36	0
58	MG	2A	3207	1/1	0.87	0.30	58,58,58,58	0
58	MG	1A	3156	1/1	0.87	0.16	24,24,24,24	0
58	MG	2T	202	1/1	0.87	0.12	65,65,65,65	0
58	MG	1A	4081	1/1	0.87	0.16	56,56,56,56	0
58	MG	2T	204	1/1	0.87	0.11	51,51,51,51	0
58	MG	1A	4086	1/1	0.87	0.18	54,54,54,54	0
58	MG	1F	306	1/1	0.87	0.11	28,28,28,28	0
58	MG	1A	3958	1/1	0.87	0.21	43,43,43,43	0
58	MG	2A	3619	1/1	0.87	0.12	39,39,39,39	0
58	MG	1a	1654	1/1	0.87	0.10	53,53,53,53	0
58	MG	2A	3784	1/1	0.87	0.22	61,61,61,61	0
58	MG	2A	3623	1/1	0.87	0.26	34,34,34,34	0
58	MG	2A	3626	1/1	0.87	0.23	60,60,60,60	0
58	MG	19	101	1/1	0.87	0.16	52,52,52,52	0
58	MG	2A	3789	1/1	0.87	0.19	67,67,67,67	0
58	MG	2A	3221	1/1	0.87	0.17	34,34,34,34	0
58	MG	1F	310	1/1	0.87	0.22	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	3476	1/1	0.87	0.15	50,50,50,50	0
58	MG	1A	3261	1/1	0.87	0.15	48,48,48,48	0
58	MG	2A	3794	1/1	0.87	0.15	52,52,52,52	0
58	MG	2A	3375	1/1	0.87	0.16	70,70,70,70	0
58	MG	1a	1792	1/1	0.87	0.10	79,79,79,79	0
58	MG	2A	3042	1/1	0.87	0.13	51,51,51,51	0
58	MG	2A	3654	1/1	0.87	0.10	68,68,68,68	0
58	MG	1A	3194	1/1	0.87	0.41	51,51,51,51	0
58	MG	2A	3302	1/1	0.87	0.32	58,58,58,58	0
58	MG	1A	3117	1/1	0.87	0.30	39,39,39,39	0
58	MG	2A	3494	1/1	0.87	0.22	58,58,58,58	0
58	MG	2A	3155	1/1	0.87	0.23	33,33,33,33	0
58	MG	1A	3320	1/1	0.87	0.18	26,26,26,26	0
58	MG	2A	3672	1/1	0.87	0.17	64,64,64,64	0
58	MG	1A	3485	1/1	0.87	0.16	35,35,35,35	0
58	MG	2A	3387	1/1	0.87	0.17	64,64,64,64	0
58	MG	2a	1631	1/1	0.87	0.16	64,64,64,64	0
58	MG	1A	3851	1/1	0.87	0.15	44,44,44,44	0
58	MG	2A	3162	1/1	0.87	0.10	58,58,58,58	0
58	MG	2A	3685	1/1	0.87	0.22	59,59,59,59	0
58	MG	2a	1636	1/1	0.87	0.22	64,64,64,64	0
58	MG	2A	3312	1/1	0.87	0.26	54,54,54,54	0
58	MG	2a	1766	1/1	0.87	0.11	65,65,65,65	0
58	MG	2A	3397	1/1	0.87	0.23	46,46,46,46	0
58	MG	2a	1771	1/1	0.87	0.13	52,52,52,52	0
58	MG	1A	4028	1/1	0.87	0.12	19,19,19,19	0
58	MG	1A	3266	1/1	0.87	0.24	41,41,41,41	0
58	MG	1A	3769	1/1	0.87	0.18	34,34,34,34	0
58	MG	1A	3556	1/1	0.87	0.19	40,40,40,40	0
58	MG	2A	3520	1/1	0.87	0.16	39,39,39,39	0
58	MG	1A	3709	1/1	0.87	0.16	54,54,54,54	0
58	MG	2a	1789	1/1	0.87	0.20	60,60,60,60	0
58	MG	2a	1646	1/1	0.87	0.14	66,66,66,66	0
58	MG	2A	3071	1/1	0.87	0.14	59,59,59,59	0
58	MG	2A	3848	1/1	0.87	0.23	59,59,59,59	0
58	MG	1A	3201	1/1	0.87	0.11	47,47,47,47	0
58	MG	1A	3527	1/1	0.87	0.22	37,37,37,37	0
58	MG	10	102	1/1	0.87	0.13	45,45,45,45	0
58	MG	1A	3217	1/1	0.87	0.28	40,40,40,40	0
58	MG	1A	3227	1/1	0.87	0.13	24,24,24,24	0
58	MG	1a	1683	1/1	0.87	0.12	57,57,57,57	0
58	MG	1A	3275	1/1	0.87	0.26	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3424	1/1	0.87	0.20	45,45,45,45	0
58	MG	2A	3725	1/1	0.87	0.10	54,54,54,54	0
58	MG	1B	217	1/1	0.87	0.15	50,50,50,50	0
58	MG	2A	3560	1/1	0.87	0.14	34,34,34,34	0
58	MG	1A	3253	1/1	0.87	0.17	48,48,48,48	0
58	MG	2a	1814	1/1	0.87	0.12	52,52,52,52	0
58	MG	1A	3615	1/1	0.87	0.14	31,31,31,31	0
58	MG	2A	3102	1/1	0.87	0.19	50,50,50,50	0
58	MG	1A	3686	1/1	0.87	0.11	27,27,27,27	0
58	MG	2A	3190	1/1	0.87	0.12	49,49,49,49	0
58	MG	1A	3730	1/1	0.87	0.15	59,59,59,59	0
58	MG	2l	201	1/1	0.87	0.17	66,66,66,66	0
58	MG	1A	3895	1/1	0.87	0.19	23,23,23,23	0
58	MG	2A	3584	1/1	0.87	0.14	34,34,34,34	0
58	MG	2A	3112	1/1	0.87	0.18	29,29,29,29	0
58	MG	2q	202	1/1	0.87	0.11	71,71,71,71	0
58	MG	2t	202	1/1	0.87	0.11	48,48,48,48	0
58	MG	1A	3138	1/1	0.87	0.17	29,29,29,29	0
58	MG	2A	3753	1/1	0.87	0.17	41,41,41,41	0
58	MG	2w	101	1/1	0.87	0.71	52,52,52,52	0
58	MG	1a	1695	1/1	0.87	0.12	55,55,55,55	0
58	MG	1a	1696	1/1	0.87	0.23	56,56,56,56	0
58	MG	2A	3449	1/1	0.87	0.38	39,39,39,39	0
58	MG	1A	4071	1/1	0.87	0.16	40,40,40,40	0
58	MG	2A	3353	1/1	0.87	0.33	71,71,71,71	0
58	MG	2A	3765	1/1	0.87	0.09	45,45,45,45	0
58	MG	1E	309	1/1	0.87	0.22	32,32,32,32	0
58	MG	1A	3216	1/1	0.88	0.25	45,45,45,45	0
58	MG	2A	3510	1/1	0.88	0.12	63,63,63,63	0
58	MG	1A	3801	1/1	0.88	0.18	31,31,31,31	0
58	MG	1A	3803	1/1	0.88	0.20	39,39,39,39	0
58	MG	1A	3512	1/1	0.88	0.18	27,27,27,27	0
58	MG	1A	3807	1/1	0.88	0.14	46,46,46,46	0
58	MG	2A	3086	1/1	0.88	0.19	68,68,68,68	0
58	MG	2A	3223	1/1	0.88	0.18	66,66,66,66	0
58	MG	1A	3808	1/1	0.88	0.13	21,21,21,21	0
58	MG	1A	3451	1/1	0.88	0.30	54,54,54,54	0
58	MG	2A	3226	1/1	0.88	0.30	49,49,49,49	0
58	MG	1A	3815	1/1	0.88	0.17	34,34,34,34	0
58	MG	2A	3536	1/1	0.88	0.16	47,47,47,47	0
58	MG	1U	206	1/1	0.88	0.28	44,44,44,44	0
58	MG	1V	204	1/1	0.88	0.34	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3951	1/1	0.88	0.07	54,54,54,54	0
58	MG	1A	4052	1/1	0.88	0.16	47,47,47,47	0
58	MG	1A	3318	1/1	0.88	0.18	52,52,52,52	0
58	MG	1A	4056	1/1	0.88	0.07	31,31,31,31	0
58	MG	2A	3107	1/1	0.88	0.09	62,62,62,62	0
58	MG	1A	3455	1/1	0.88	0.24	46,46,46,46	0
58	MG	1A	3954	1/1	0.88	0.15	53,53,53,53	0
58	MG	1A	3521	1/1	0.88	0.19	68,68,68,68	0
58	MG	2A	3570	1/1	0.88	0.17	67,67,67,67	0
58	MG	2A	3571	1/1	0.88	0.23	56,56,56,56	0
58	MG	2A	3573	1/1	0.88	0.11	45,45,45,45	0
58	MG	1A	3319	1/1	0.88	0.17	36,36,36,36	0
58	MG	1A	3077	1/1	0.88	0.22	45,45,45,45	0
58	MG	2A	3118	1/1	0.88	0.15	60,60,60,60	0
58	MG	2A	3119	1/1	0.88	0.10	55,55,55,55	0
58	MG	2A	3250	1/1	0.88	0.20	57,57,57,57	0
58	MG	2A	3585	1/1	0.88	0.15	59,59,59,59	0
58	MG	2a	1682	1/1	0.88	0.27	60,60,60,60	0
58	MG	1A	3525	1/1	0.88	0.31	43,43,43,43	0
58	MG	1A	4076	1/1	0.88	0.20	36,36,36,36	0
58	MG	2A	3817	1/1	0.88	0.19	45,45,45,45	0
58	MG	1A	3460	1/1	0.88	0.35	40,40,40,40	0
58	MG	2A	3820	1/1	0.88	0.15	50,50,50,50	0
58	MG	1A	4082	1/1	0.88	0.27	56,56,56,56	0
58	MG	2A	3256	1/1	0.88	0.09	42,42,42,42	0
58	MG	1a	1686	1/1	0.88	0.14	59,59,59,59	0
58	MG	1A	3092	1/1	0.88	0.18	54,54,54,54	0
58	MG	2A	3259	1/1	0.88	0.37	68,68,68,68	0
58	MG	2A	3391	1/1	0.88	0.19	59,59,59,59	0
58	MG	2A	3392	1/1	0.88	0.19	52,52,52,52	0
58	MG	2A	3394	1/1	0.88	0.25	54,54,54,54	0
58	MG	2A	3613	1/1	0.88	0.15	35,35,35,35	0
58	MG	1A	3361	1/1	0.88	0.25	56,56,56,56	0
58	MG	1A	3229	1/1	0.88	0.17	40,40,40,40	0
58	MG	2a	1711	1/1	0.88	0.17	60,60,60,60	0
58	MG	2A	3840	1/1	0.88	0.19	54,54,54,54	0
58	MG	2A	3844	1/1	0.88	0.10	59,59,59,59	0
58	MG	2A	3138	1/1	0.88	0.24	53,53,53,53	0
58	MG	2A	3404	1/1	0.88	0.22	63,63,63,63	0
58	MG	2a	1716	1/1	0.88	0.27	53,53,53,53	0
58	MG	2B	203	1/1	0.88	0.10	72,72,72,72	0
58	MG	1A	3364	1/1	0.88	0.17	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	4094	1/1	0.88	0.26	52,52,52,52	0
58	MG	18	102	1/1	0.88	0.31	36,36,36,36	0
58	MG	2A	3267	1/1	0.88	0.24	64,64,64,64	0
58	MG	2A	3636	1/1	0.88	0.21	48,48,48,48	0
58	MG	2a	1731	1/1	0.88	0.35	64,64,64,64	0
58	MG	2a	1734	1/1	0.88	0.34	67,67,67,67	0
58	MG	1A	3969	1/1	0.88	0.30	53,53,53,53	0
58	MG	2B	212	1/1	0.88	0.21	61,61,61,61	0
58	MG	2A	3639	1/1	0.88	0.20	41,41,41,41	0
58	MG	1A	3272	1/1	0.88	0.15	46,46,46,46	0
58	MG	2a	1741	1/1	0.88	0.22	63,63,63,63	0
58	MG	1l	201	1/1	0.88	0.21	66,66,66,66	0
58	MG	2A	3642	1/1	0.88	0.14	65,65,65,65	0
58	MG	1A	3867	1/1	0.88	0.13	38,38,38,38	0
58	MG	2A	3416	1/1	0.88	0.19	56,56,56,56	0
58	MG	2a	1747	1/1	0.88	0.14	63,63,63,63	0
58	MG	2A	3153	1/1	0.88	0.17	57,57,57,57	0
58	MG	1A	3329	1/1	0.88	0.23	45,45,45,45	0
58	MG	2A	3653	1/1	0.88	0.14	51,51,51,51	0
58	MG	1A	3231	1/1	0.88	0.24	40,40,40,40	0
58	MG	1A	3979	1/1	0.88	0.10	59,59,59,59	0
58	MG	2A	3157	1/1	0.88	0.10	45,45,45,45	0
58	MG	1a	1700	1/1	0.88	0.39	45,45,45,45	0
58	MG	2A	3426	1/1	0.88	0.21	50,50,50,50	0
58	MG	1x	102	1/1	0.88	0.28	70,70,70,70	0
58	MG	2A	3428	1/1	0.88	0.24	51,51,51,51	0
58	MG	1A	3875	1/1	0.88	0.44	35,35,35,35	0
58	MG	2A	3284	1/1	0.88	0.32	56,56,56,56	0
58	MG	1B	208	1/1	0.88	0.10	60,60,60,60	0
58	MG	1A	3981	1/1	0.88	0.17	56,56,56,56	0
58	MG	2A	3679	1/1	0.88	0.19	52,52,52,52	0
58	MG	1A	3884	1/1	0.88	0.07	57,57,57,57	0
58	MG	2a	1772	1/1	0.88	0.21	48,48,48,48	0
58	MG	1A	3623	1/1	0.88	0.20	37,37,37,37	0
58	MG	1A	3334	1/1	0.88	0.20	55,55,55,55	0
58	MG	1A	3335	1/1	0.88	0.27	57,57,57,57	0
58	MG	1x	112	1/1	0.88	0.11	58,58,58,58	0
58	MG	2A	3297	1/1	0.88	0.25	63,63,63,63	0
58	MG	1A	3433	1/1	0.88	0.17	43,43,43,43	0
58	MG	1a	1719	1/1	0.88	0.18	54,54,54,54	0
58	MG	1A	3643	1/1	0.88	0.13	46,46,46,46	0
58	MG	2A	3703	1/1	0.88	0.22	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	3338	1/1	0.88	0.23	53,53,53,53	0
58	MG	2A	3304	1/1	0.88	0.23	49,49,49,49	0
58	MG	25	102	1/1	0.88	0.14	43,43,43,43	0
58	MG	1B	221	1/1	0.88	0.23	45,45,45,45	0
58	MG	1A	4003	1/1	0.88	0.09	62,62,62,62	0
58	MG	2A	3018	1/1	0.88	0.13	64,64,64,64	0
58	MG	1A	3256	1/1	0.88	0.11	62,62,62,62	0
58	MG	1A	3761	1/1	0.88	0.27	51,51,51,51	0
58	MG	2A	3718	1/1	0.88	0.17	62,62,62,62	0
58	MG	1A	3437	1/1	0.88	0.16	56,56,56,56	0
58	MG	2A	3187	1/1	0.88	0.22	59,59,59,59	0
58	MG	1B	229	1/1	0.88	0.22	41,41,41,41	0
58	MG	2a	1811	1/1	0.88	0.14	57,57,57,57	0
58	MG	1B	235	1/1	0.88	0.34	70,70,70,70	0
58	MG	1A	3073	1/1	0.88	0.17	12,12,12,12	0
58	MG	2a	1818	1/1	0.88	0.26	54,54,54,54	0
58	MG	2A	3194	1/1	0.88	0.10	53,53,53,53	0
58	MG	2A	3318	1/1	0.88	0.45	66,66,66,66	0
58	MG	1A	3097	1/1	0.88	0.13	28,28,28,28	0
58	MG	2A	3483	1/1	0.88	0.16	40,40,40,40	0
58	MG	1A	3016	1/1	0.88	0.19	52,52,52,52	0
58	MG	2A	3743	1/1	0.88	0.13	59,59,59,59	0
58	MG	2A	3488	1/1	0.88	0.08	61,61,61,61	0
58	MG	1A	3026	1/1	0.88	0.22	51,51,51,51	0
58	MG	2A	3198	1/1	0.88	0.28	51,51,51,51	0
58	MG	1a	1747	1/1	0.88	0.15	66,66,66,66	0
58	MG	2A	3749	1/1	0.88	0.20	49,49,49,49	0
58	MG	1A	3500	1/1	0.88	0.33	56,56,56,56	0
58	MG	2v	102	1/1	0.88	0.10	68,68,68,68	0
58	MG	2a	1630	1/1	0.88	0.19	71,71,71,71	0
58	MG	2v	104	1/1	0.88	0.21	62,62,62,62	0
58	MG	1A	3443	1/1	0.88	0.13	31,31,31,31	0
58	MG	1A	3569	1/1	0.88	0.16	30,30,30,30	0
58	MG	2A	3755	1/1	0.88	0.23	53,53,53,53	0
58	MG	2A	3206	1/1	0.88	0.28	53,53,53,53	0
58	MG	1A	3578	1/1	0.88	0.17	29,29,29,29	0
58	MG	1A	3928	1/1	0.88	0.20	55,55,55,55	0
58	MG	1A	3352	1/1	0.88	0.17	62,62,62,62	0
58	MG	1A	3587	1/1	0.88	0.27	43,43,43,43	0
58	MG	2A	3566	1/1	0.89	0.14	39,39,39,39	0
58	MG	1A	3321	1/1	0.89	0.21	50,50,50,50	0
58	MG	1A	3857	1/1	0.89	0.23	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	1754	1/1	0.89	0.13	52,52,52,52	0
58	MG	1A	3373	1/1	0.89	0.18	47,47,47,47	0
58	MG	1A	3107	1/1	0.89	0.20	24,24,24,24	0
58	MG	1A	3009	1/1	0.89	0.17	24,24,24,24	0
58	MG	2A	3097	1/1	0.89	0.11	55,55,55,55	0
58	MG	1A	3379	1/1	0.89	0.18	47,47,47,47	0
58	MG	2A	3581	1/1	0.89	0.21	58,58,58,58	0
58	MG	2A	3381	1/1	0.89	0.09	57,57,57,57	0
58	MG	1A	3289	1/1	0.89	0.22	54,54,54,54	0
58	MG	1A	3995	1/1	0.89	0.15	45,45,45,45	0
58	MG	2a	1667	1/1	0.89	0.14	51,51,51,51	0
58	MG	2A	3589	1/1	0.89	0.16	36,36,36,36	0
58	MG	2A	3590	1/1	0.89	0.11	34,34,34,34	0
58	MG	2A	3593	1/1	0.89	0.09	50,50,50,50	0
58	MG	1A	3520	1/1	0.89	0.18	55,55,55,55	0
58	MG	1a	1767	1/1	0.89	0.07	54,54,54,54	0
58	MG	1A	3883	1/1	0.89	0.12	36,36,36,36	0
58	MG	2A	3601	1/1	0.89	0.34	58,58,58,58	0
58	MG	1A	3388	1/1	0.89	0.21	31,31,31,31	0
58	MG	1A	3522	1/1	0.89	0.30	60,60,60,60	0
58	MG	1A	3175	1/1	0.89	0.15	26,26,26,26	0
58	MG	1a	1773	1/1	0.89	0.06	38,38,38,38	0
58	MG	1A	3605	1/1	0.89	0.36	47,47,47,47	0
58	MG	1A	3292	1/1	0.89	0.26	32,32,32,32	0
58	MG	2A	3120	1/1	0.89	0.46	53,53,53,53	0
58	MG	2a	1689	1/1	0.89	0.25	67,67,67,67	0
58	MG	2A	3612	1/1	0.89	0.19	53,53,53,53	0
58	MG	2A	3121	1/1	0.89	0.16	44,44,44,44	0
58	MG	2A	3832	1/1	0.89	0.20	54,54,54,54	0
58	MG	1B	231	1/1	0.89	0.21	66,66,66,66	0
58	MG	2a	1697	1/1	0.89	0.44	63,63,63,63	0
58	MG	1a	1644	1/1	0.89	0.12	41,41,41,41	0
58	MG	1A	3394	1/1	0.89	0.14	45,45,45,45	0
58	MG	1A	3176	1/1	0.89	0.26	19,19,19,19	0
58	MG	2A	3838	1/1	0.89	0.14	60,60,60,60	0
58	MG	1A	4018	1/1	0.89	0.12	49,49,49,49	0
58	MG	1A	3078	1/1	0.89	0.16	30,30,30,30	0
58	MG	2A	3625	1/1	0.89	0.13	38,38,38,38	0
58	MG	1A	3531	1/1	0.89	0.29	51,51,51,51	0
58	MG	2B	201	1/1	0.89	0.12	59,59,59,59	0
58	MG	1A	3400	1/1	0.89	0.15	35,35,35,35	0
58	MG	2A	3415	1/1	0.89	0.37	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3756	1/1	0.89	0.17	37,37,37,37	0
58	MG	1A	3898	1/1	0.89	0.15	26,26,26,26	0
58	MG	1A	4025	1/1	0.89	0.12	34,34,34,34	0
58	MG	1A	3759	1/1	0.89	0.27	29,29,29,29	0
58	MG	2A	3421	1/1	0.89	0.19	53,53,53,53	0
58	MG	2a	1722	1/1	0.89	0.34	58,58,58,58	0
58	MG	2A	3276	1/1	0.89	0.22	66,66,66,66	0
58	MG	1A	3298	1/1	0.89	0.18	28,28,28,28	0
58	MG	1G	203	1/1	0.89	0.14	61,61,61,61	0
58	MG	1A	3626	1/1	0.89	0.19	26,26,26,26	0
58	MG	1A	3631	1/1	0.89	0.24	61,61,61,61	0
58	MG	1O	204	1/1	0.89	0.30	43,43,43,43	0
58	MG	1A	4030	1/1	0.89	0.16	46,46,46,46	0
58	MG	1A	3258	1/1	0.89	0.28	37,37,37,37	0
58	MG	1A	3461	1/1	0.89	0.35	68,68,68,68	0
58	MG	1A	3404	1/1	0.89	0.30	54,54,54,54	0
58	MG	1A	3259	1/1	0.89	0.18	38,38,38,38	0
58	MG	1A	3096	1/1	0.89	0.17	40,40,40,40	0
58	MG	1f	201	1/1	0.89	0.17	47,47,47,47	0
58	MG	1A	3775	1/1	0.89	0.17	22,22,22,22	0
58	MG	2E	305	1/1	0.89	0.17	35,35,35,35	0
58	MG	2a	1746	1/1	0.89	0.15	66,66,66,66	0
58	MG	2A	3295	1/1	0.89	0.19	46,46,46,46	0
58	MG	1A	3933	1/1	0.89	0.13	36,36,36,36	0
58	MG	1A	3653	1/1	0.89	0.18	29,29,29,29	0
58	MG	1A	4045	1/1	0.89	0.18	43,43,43,43	0
58	MG	2A	3451	1/1	0.89	0.18	40,40,40,40	0
58	MG	2a	1752	1/1	0.89	0.14	69,69,69,69	0
58	MG	1A	4047	1/1	0.89	0.15	25,25,25,25	0
58	MG	1A	3224	1/1	0.89	0.31	47,47,47,47	0
58	MG	2A	3690	1/1	0.89	0.30	75,75,75,75	0
58	MG	1A	4049	1/1	0.89	0.34	62,62,62,62	0
58	MG	1A	4051	1/1	0.89	0.21	59,59,59,59	0
58	MG	10	105	1/1	0.89	0.25	58,58,58,58	0
58	MG	1A	3783	1/1	0.89	0.14	24,24,24,24	0
58	MG	1A	3347	1/1	0.89	0.22	58,58,58,58	0
58	MG	2A	3467	1/1	0.89	0.12	49,49,49,49	0
58	MG	10	109	1/1	0.89	0.12	53,53,53,53	0
58	MG	1A	3546	1/1	0.89	0.21	59,59,59,59	0
58	MG	2A	3180	1/1	0.89	0.30	67,67,67,67	0
58	MG	1A	3005	1/1	0.89	0.17	32,32,32,32	0
58	MG	2A	3474	1/1	0.89	0.18	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3182	1/1	0.89	0.19	60,60,60,60	0
58	MG	1A	3798	1/1	0.89	0.09	32,32,32,32	0
58	MG	2a	1778	1/1	0.89	0.17	67,67,67,67	0
58	MG	1A	4060	1/1	0.89	0.16	45,45,45,45	0
58	MG	2a	1783	1/1	0.89	0.21	69,69,69,69	0
58	MG	1A	3100	1/1	0.89	0.20	61,61,61,61	0
58	MG	1A	3552	1/1	0.89	0.39	49,49,49,49	0
58	MG	1A	3411	1/1	0.89	0.14	43,43,43,43	0
58	MG	2A	3009	1/1	0.89	0.25	55,55,55,55	0
58	MG	2A	3191	1/1	0.89	0.16	43,43,43,43	0
58	MG	2A	3727	1/1	0.89	0.08	63,63,63,63	0
58	MG	2a	1604	1/1	0.89	0.21	71,71,71,71	0
58	MG	2A	3192	1/1	0.89	0.12	48,48,48,48	0
58	MG	2a	1606	1/1	0.89	0.17	59,59,59,59	0
58	MG	1a	1706	1/1	0.89	0.14	63,63,63,63	0
58	MG	2A	3735	1/1	0.89	0.19	62,62,62,62	0
58	MG	2A	3016	1/1	0.89	0.28	51,51,51,51	0
58	MG	1A	4072	1/1	0.89	0.14	44,44,44,44	0
58	MG	1A	3805	1/1	0.89	0.14	64,64,64,64	0
58	MG	1a	1710	1/1	0.89	0.19	53,53,53,53	0
58	MG	15	104	1/1	0.89	0.18	26,26,26,26	0
58	MG	1A	3185	1/1	0.89	0.39	40,40,40,40	0
58	MG	1A	4077	1/1	0.89	0.18	30,30,30,30	0
58	MG	2A	3335	1/1	0.89	0.39	73,73,73,73	0
58	MG	1A	3233	1/1	0.89	0.40	44,44,44,44	0
58	MG	2a	1815	1/1	0.89	0.19	61,61,61,61	0
58	MG	2a	1816	1/1	0.89	0.25	65,65,65,65	0
58	MG	1A	3311	1/1	0.89	0.14	63,63,63,63	0
58	MG	1A	3422	1/1	0.89	0.15	44,44,44,44	0
58	MG	1A	3152	1/1	0.89	0.64	42,42,42,42	0
58	MG	2A	3754	1/1	0.89	0.47	48,48,48,48	0
58	MG	2A	3044	1/1	0.89	0.11	49,49,49,49	0
58	MG	2j	201	1/1	0.89	0.20	59,59,59,59	0
58	MG	2A	3517	1/1	0.89	0.16	58,58,58,58	0
58	MG	1A	3359	1/1	0.89	0.11	59,59,59,59	0
58	MG	2l	202	1/1	0.89	0.26	59,59,59,59	0
58	MG	1A	3823	1/1	0.89	0.16	39,39,39,39	0
58	MG	2A	3347	1/1	0.89	0.14	65,65,65,65	0
58	MG	1A	4092	1/1	0.89	0.29	56,56,56,56	0
58	MG	2A	3054	1/1	0.89	0.11	63,63,63,63	0
58	MG	1A	3155	1/1	0.89	0.16	39,39,39,39	0
58	MG	1A	3571	1/1	0.89	0.34	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	1604	1/1	0.89	0.11	51,51,51,51	0
58	MG	1A	3697	1/1	0.89	0.11	27,27,27,27	0
58	MG	1A	3842	1/1	0.89	0.12	49,49,49,49	0
58	MG	1A	4100	1/1	0.89	0.10	41,41,41,41	0
58	MG	2A	3362	1/1	0.89	0.18	49,49,49,49	0
58	MG	2A	3067	1/1	0.89	0.16	51,51,51,51	0
58	MG	1A	3103	1/1	0.89	0.20	35,35,35,35	0
58	MG	2x	103	1/1	0.89	0.14	53,53,53,53	0
58	MG	1A	3091	1/1	0.89	0.20	40,40,40,40	0
58	MG	1B	202	1/1	0.89	0.22	52,52,52,52	0
59	K	2A	3443	1/1	0.89	0.13	51,51,51,51	0
58	MG	1A	3283	1/1	0.89	0.20	35,35,35,35	0
58	MG	1A	3129	1/1	0.89	0.26	37,37,37,37	0
58	MG	2A	3600	1/1	0.90	0.16	58,58,58,58	0
58	MG	1A	3788	1/1	0.90	0.12	59,59,59,59	0
58	MG	1A	3483	1/1	0.90	0.26	52,52,52,52	0
58	MG	2A	3288	1/1	0.90	0.09	52,52,52,52	0
58	MG	1A	3022	1/1	0.90	0.15	38,38,38,38	0
58	MG	1A	3796	1/1	0.90	0.20	60,60,60,60	0
58	MG	2A	3420	1/1	0.90	0.32	49,49,49,49	0
58	MG	2A	3004	1/1	0.90	0.29	45,45,45,45	0
58	MG	2A	3422	1/1	0.90	0.10	63,63,63,63	0
58	MG	1A	3313	1/1	0.90	0.13	45,45,45,45	0
58	MG	1A	3487	1/1	0.90	0.18	42,42,42,42	0
58	MG	2A	3294	1/1	0.90	0.13	65,65,65,65	0
58	MG	1A	3180	1/1	0.90	0.16	48,48,48,48	0
58	MG	2A	3014	1/1	0.90	0.32	38,38,38,38	0
58	MG	1A	3024	1/1	0.90	0.22	45,45,45,45	0
58	MG	1A	3616	1/1	0.90	0.21	52,52,52,52	0
58	MG	2A	3430	1/1	0.90	0.20	54,54,54,54	0
58	MG	1A	3153	1/1	0.90	0.11	39,39,39,39	0
58	MG	2A	3835	1/1	0.90	0.18	60,60,60,60	0
58	MG	1A	3254	1/1	0.90	0.16	19,19,19,19	0
58	MG	2A	3627	1/1	0.90	0.26	55,55,55,55	0
58	MG	1a	1609	1/1	0.90	0.14	57,57,57,57	0
58	MG	2A	3437	1/1	0.90	0.09	53,53,53,53	0
58	MG	2A	3438	1/1	0.90	0.14	33,33,33,33	0
58	MG	2A	3303	1/1	0.90	0.27	56,56,56,56	0
58	MG	2A	3845	1/1	0.90	0.17	63,63,63,63	0
58	MG	2a	1699	1/1	0.90	0.10	70,70,70,70	0
58	MG	1A	3936	1/1	0.90	0.13	33,33,33,33	0
58	MG	2A	3851	1/1	0.90	0.13	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1a	1612	1/1	0.90	0.10	57,57,57,57	0
58	MG	1A	3403	1/1	0.90	0.16	40,40,40,40	0
58	MG	2A	3446	1/1	0.90	0.28	57,57,57,57	0
58	MG	2A	3645	1/1	0.90	0.22	66,66,66,66	0
58	MG	1A	3811	1/1	0.90	0.11	22,22,22,22	0
58	MG	1a	1737	1/1	0.90	0.14	71,71,71,71	0
58	MG	1A	3219	1/1	0.90	0.17	37,37,37,37	0
58	MG	2A	3041	1/1	0.90	0.60	54,54,54,54	0
58	MG	1a	1620	1/1	0.90	0.12	38,38,38,38	0
58	MG	2A	3655	1/1	0.90	0.30	65,65,65,65	0
58	MG	1B	230	1/1	0.90	0.17	40,40,40,40	0
58	MG	2a	1717	1/1	0.90	0.36	58,58,58,58	0
58	MG	2A	3456	1/1	0.90	0.09	54,54,54,54	0
58	MG	1A	3629	1/1	0.90	0.15	46,46,46,46	0
58	MG	1A	3944	1/1	0.90	0.08	33,33,33,33	0
58	MG	2A	3667	1/1	0.90	0.13	51,51,51,51	0
58	MG	1A	3444	1/1	0.90	0.27	41,41,41,41	0
58	MG	1A	3220	1/1	0.90	0.14	41,41,41,41	0
58	MG	1a	1748	1/1	0.90	0.18	36,36,36,36	0
58	MG	2A	3200	1/1	0.90	0.28	71,71,71,71	0
58	MG	1A	3723	1/1	0.90	0.11	36,36,36,36	0
58	MG	2A	3058	1/1	0.90	0.16	38,38,38,38	0
58	MG	1A	3503	1/1	0.90	0.24	54,54,54,54	0
58	MG	2a	1737	1/1	0.90	0.25	62,62,62,62	0
58	MG	2a	1738	1/1	0.90	0.16	53,53,53,53	0
58	MG	1A	3637	1/1	0.90	0.14	27,27,27,27	0
58	MG	1a	1753	1/1	0.90	0.14	49,49,49,49	0
58	MG	2E	310	1/1	0.90	0.24	41,41,41,41	0
58	MG	2A	3208	1/1	0.90	0.20	60,60,60,60	0
58	MG	1A	3257	1/1	0.90	0.17	26,26,26,26	0
58	MG	2A	3331	1/1	0.90	0.11	70,70,70,70	0
58	MG	2A	3478	1/1	0.90	0.18	54,54,54,54	0
58	MG	2G	201	1/1	0.90	0.22	62,62,62,62	0
58	MG	2A	3479	1/1	0.90	0.15	52,52,52,52	0
58	MG	1A	4043	1/1	0.90	0.22	42,42,42,42	0
58	MG	2Q	201	1/1	0.90	0.14	53,53,53,53	0
58	MG	2A	3698	1/1	0.90	0.10	61,61,61,61	0
58	MG	1A	3739	1/1	0.90	0.15	56,56,56,56	0
58	MG	1F	308	1/1	0.90	0.17	31,31,31,31	0
58	MG	2A	3076	1/1	0.90	0.14	46,46,46,46	0
58	MG	1A	3846	1/1	0.90	0.22	71,71,71,71	0
58	MG	2A	3215	1/1	0.90	0.19	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3489	1/1	0.90	0.21	53,53,53,53	0
58	MG	1A	3045	1/1	0.90	0.24	34,34,34,34	0
58	MG	1F	312	1/1	0.90	0.13	42,42,42,42	0
58	MG	2A	3492	1/1	0.90	0.16	42,42,42,42	0
58	MG	2V	201	1/1	0.90	0.33	45,45,45,45	0
58	MG	1G	201	1/1	0.90	0.20	40,40,40,40	0
58	MG	1G	202	1/1	0.90	0.23	63,63,63,63	0
58	MG	1A	3510	1/1	0.90	0.26	54,54,54,54	0
58	MG	1A	3324	1/1	0.90	0.22	55,55,55,55	0
58	MG	23	102	1/1	0.90	0.19	48,48,48,48	0
58	MG	25	101	1/1	0.90	0.20	46,46,46,46	0
58	MG	1A	3060	1/1	0.90	0.28	48,48,48,48	0
58	MG	1A	3746	1/1	0.90	0.13	45,45,45,45	0
58	MG	27	102	1/1	0.90	0.17	52,52,52,52	0
58	MG	1A	3862	1/1	0.90	0.18	47,47,47,47	0
58	MG	1A	3049	1/1	0.90	0.17	19,19,19,19	0
58	MG	1A	3755	1/1	0.90	0.18	61,61,61,61	0
58	MG	1A	3328	1/1	0.90	0.22	42,42,42,42	0
58	MG	2a	1788	1/1	0.90	0.12	66,66,66,66	0
58	MG	1a	1657	1/1	0.90	0.09	41,41,41,41	0
58	MG	1R	203	1/1	0.90	0.18	33,33,33,33	0
58	MG	2a	1791	1/1	0.90	0.12	75,75,75,75	0
58	MG	1A	3869	1/1	0.90	0.26	63,63,63,63	0
58	MG	1A	3970	1/1	0.90	0.17	42,42,42,42	0
58	MG	2A	3365	1/1	0.90	0.17	66,66,66,66	0
58	MG	1A	4069	1/1	0.90	0.21	32,32,32,32	0
58	MG	1A	3670	1/1	0.90	0.15	35,35,35,35	0
58	MG	2a	1800	1/1	0.90	0.29	57,57,57,57	0
58	MG	2A	3521	1/1	0.90	0.17	40,40,40,40	0
58	MG	1a	1664	1/1	0.90	0.16	50,50,50,50	0
58	MG	1A	3872	1/1	0.90	0.15	42,42,42,42	0
58	MG	1A	3760	1/1	0.90	0.15	53,53,53,53	0
58	MG	2a	1806	1/1	0.90	0.16	68,68,68,68	0
58	MG	1a	1794	1/1	0.90	0.13	60,60,60,60	0
58	MG	1X	101	1/1	0.90	0.20	34,34,34,34	0
58	MG	2A	3535	1/1	0.90	0.26	62,62,62,62	0
58	MG	1Y	201	1/1	0.90	0.18	49,49,49,49	0
58	MG	1A	3159	1/1	0.90	0.21	31,31,31,31	0
58	MG	1Z	301	1/1	0.90	0.23	43,43,43,43	0
58	MG	2A	3545	1/1	0.90	0.09	46,46,46,46	0
58	MG	2A	3550	1/1	0.90	0.28	51,51,51,51	0
58	MG	1A	3877	1/1	0.90	0.12	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3133	1/1	0.90	0.13	54,54,54,54	0
58	MG	1A	3066	1/1	0.90	0.30	47,47,47,47	0
58	MG	1A	3235	1/1	0.90	0.39	32,32,32,32	0
58	MG	1A	3067	1/1	0.90	0.20	26,26,26,26	0
58	MG	1A	3984	1/1	0.90	0.22	23,23,23,23	0
58	MG	1A	3337	1/1	0.90	0.40	61,61,61,61	0
58	MG	2A	3385	1/1	0.90	0.11	56,56,56,56	0
58	MG	2A	3568	1/1	0.90	0.15	56,56,56,56	0
58	MG	1A	4089	1/1	0.90	0.36	50,50,50,50	0
58	MG	1A	3469	1/1	0.90	0.24	53,53,53,53	0
58	MG	1A	3382	1/1	0.90	0.21	48,48,48,48	0
58	MG	2A	3572	1/1	0.90	0.24	44,44,44,44	0
58	MG	1l	104	1/1	0.90	0.12	44,44,44,44	0
58	MG	2q	203	1/1	0.90	0.21	70,70,70,70	0
58	MG	1f	202	1/1	0.90	0.35	60,60,60,60	0
58	MG	1A	3990	1/1	0.90	0.12	50,50,50,50	0
58	MG	1A	4095	1/1	0.90	0.21	57,57,57,57	0
58	MG	1A	3139	1/1	0.90	0.24	53,53,53,53	0
58	MG	1A	3430	1/1	0.90	0.10	59,59,59,59	0
58	MG	1A	3998	1/1	0.90	0.15	19,19,19,19	0
58	MG	1A	3015	1/1	0.90	0.24	32,32,32,32	0
58	MG	1A	4001	1/1	0.90	0.12	59,59,59,59	0
58	MG	1A	3780	1/1	0.90	0.12	57,57,57,57	0
58	MG	1A	3690	1/1	0.90	0.12	27,27,27,27	0
58	MG	1B	203	1/1	0.90	0.23	40,40,40,40	0
58	MG	18	101	1/1	0.90	0.16	51,51,51,51	0
58	MG	1A	3147	1/1	0.90	0.20	31,31,31,31	0
58	MG	1A	3248	1/1	0.90	0.13	56,56,56,56	0
58	MG	2A	3599	1/1	0.90	0.16	56,56,56,56	0
58	MG	2A	3132	1/1	0.91	0.15	38,38,38,38	0
58	MG	2A	3680	1/1	0.91	0.11	52,52,52,52	0
58	MG	1A	3858	1/1	0.91	0.06	53,53,53,53	0
58	MG	1A	3056	1/1	0.91	0.19	30,30,30,30	0
58	MG	1B	234	1/1	0.91	0.14	41,41,41,41	0
58	MG	2A	3505	1/1	0.91	0.16	71,71,71,71	0
58	MG	1A	3384	1/1	0.91	0.23	47,47,47,47	0
58	MG	1a	1699	1/1	0.91	0.25	48,48,48,48	0
58	MG	1B	236	1/1	0.91	0.09	73,73,73,73	0
58	MG	1a	1701	1/1	0.91	0.20	47,47,47,47	0
58	MG	2A	3697	1/1	0.91	0.23	71,71,71,71	0
58	MG	1A	3865	1/1	0.91	0.12	47,47,47,47	0
58	MG	1D	307	1/1	0.91	0.28	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	1D	312	1/1	0.91	0.24	32,32,32,32	0
58	MG	1x	103	1/1	0.91	0.09	53,53,53,53	0
58	MG	1A	3505	1/1	0.91	0.19	46,46,46,46	0
58	MG	1E	301	1/1	0.91	0.19	46,46,46,46	0
58	MG	1A	3471	1/1	0.91	0.23	59,59,59,59	0
58	MG	2A	3526	1/1	0.91	0.10	38,38,38,38	0
58	MG	2A	3529	1/1	0.91	0.08	43,43,43,43	0
58	MG	2E	306	1/1	0.91	0.15	51,51,51,51	0
58	MG	1A	3001	1/1	0.91	0.15	34,34,34,34	0
58	MG	2E	309	1/1	0.91	0.09	48,48,48,48	0
58	MG	1A	3290	1/1	0.91	0.08	48,48,48,48	0
58	MG	1E	311	1/1	0.91	0.21	43,43,43,43	0
58	MG	1A	3118	1/1	0.91	0.15	29,29,29,29	0
58	MG	1A	3555	1/1	0.91	0.28	36,36,36,36	0
58	MG	2F	304	1/1	0.91	0.17	42,42,42,42	0
58	MG	2A	3722	1/1	0.91	0.29	68,68,68,68	0
58	MG	1A	3694	1/1	0.91	0.14	33,33,33,33	0
58	MG	1a	1724	1/1	0.91	0.29	50,50,50,50	0
58	MG	2O	202	1/1	0.91	0.20	54,54,54,54	0
58	MG	1A	3476	1/1	0.91	0.23	58,58,58,58	0
58	MG	2a	1732	1/1	0.91	0.23	65,65,65,65	0
58	MG	2P	202	1/1	0.91	0.14	64,64,64,64	0
58	MG	2A	3548	1/1	0.91	0.14	32,32,32,32	0
58	MG	1A	3881	1/1	0.91	0.27	42,42,42,42	0
58	MG	1A	3973	1/1	0.91	0.09	44,44,44,44	0
58	MG	2R	201	1/1	0.91	0.27	55,55,55,55	0
58	MG	1A	3610	1/1	0.91	0.23	51,51,51,51	0
58	MG	2A	3011	1/1	0.91	0.16	35,35,35,35	0
58	MG	1a	1625	1/1	0.91	0.12	58,58,58,58	0
58	MG	2A	3741	1/1	0.91	0.44	48,48,48,48	0
58	MG	1A	3205	1/1	0.91	0.22	31,31,31,31	0
58	MG	2A	3285	1/1	0.91	0.35	56,56,56,56	0
58	MG	1A	3053	1/1	0.91	0.18	41,41,41,41	0
58	MG	2A	3287	1/1	0.91	0.19	55,55,55,55	0
58	MG	1A	3417	1/1	0.91	0.35	42,42,42,42	0
58	MG	1H	201	1/1	0.91	0.28	42,42,42,42	0
58	MG	1a	1630	1/1	0.91	0.16	59,59,59,59	0
58	MG	1A	3446	1/1	0.91	0.37	28,28,28,28	0
58	MG	1A	3165	1/1	0.91	0.20	30,30,30,30	0
58	MG	1a	1634	1/1	0.91	0.22	59,59,59,59	0
58	MG	1A	3789	1/1	0.91	0.16	46,46,46,46	0
58	MG	1A	3154	1/1	0.91	0.28	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3234	1/1	0.91	0.22	56,56,56,56	0
58	MG	2A	3579	1/1	0.91	0.22	56,56,56,56	0
58	MG	1A	4080	1/1	0.91	0.21	32,32,32,32	0
58	MG	1A	3630	1/1	0.91	0.11	43,43,43,43	0
58	MG	1Q	208	1/1	0.91	0.21	42,42,42,42	0
58	MG	2A	3045	1/1	0.91	0.18	29,29,29,29	0
58	MG	1A	3713	1/1	0.91	0.22	40,40,40,40	0
58	MG	1A	3454	1/1	0.91	0.21	39,39,39,39	0
58	MG	2a	1767	1/1	0.91	0.09	61,61,61,61	0
58	MG	1A	3577	1/1	0.91	0.28	37,37,37,37	0
58	MG	2a	1769	1/1	0.91	0.20	68,68,68,68	0
58	MG	2A	3772	1/1	0.91	0.16	39,39,39,39	0
58	MG	2A	3591	1/1	0.91	0.18	63,63,63,63	0
58	MG	2A	3774	1/1	0.91	0.16	62,62,62,62	0
58	MG	1A	3992	1/1	0.91	0.14	52,52,52,52	0
58	MG	1U	204	1/1	0.91	0.15	44,44,44,44	0
58	MG	1A	3906	1/1	0.91	0.10	52,52,52,52	0
58	MG	2A	3597	1/1	0.91	0.20	67,67,67,67	0
58	MG	2a	1782	1/1	0.91	0.12	68,68,68,68	0
58	MG	2A	3433	1/1	0.91	0.28	57,57,57,57	0
58	MG	1A	3908	1/1	0.91	0.16	51,51,51,51	0
58	MG	1A	3909	1/1	0.91	0.21	24,24,24,24	0
58	MG	2a	1787	1/1	0.91	0.13	58,58,58,58	0
58	MG	2A	3061	1/1	0.91	0.26	66,66,66,66	0
58	MG	1V	207	1/1	0.91	0.18	55,55,55,55	0
58	MG	1A	3910	1/1	0.91	0.17	55,55,55,55	0
58	MG	1A	3634	1/1	0.91	0.05	33,33,33,33	0
58	MG	2a	1626	1/1	0.91	0.17	65,65,65,65	0
58	MG	1A	3142	1/1	0.91	0.14	42,42,42,42	0
58	MG	1A	3918	1/1	0.91	0.17	28,28,28,28	0
58	MG	1A	4004	1/1	0.91	0.17	31,31,31,31	0
58	MG	1A	3122	1/1	0.91	0.21	35,35,35,35	0
58	MG	2A	3077	1/1	0.91	0.08	47,47,47,47	0
58	MG	1a	1776	1/1	0.91	0.22	43,43,43,43	0
58	MG	2a	1802	1/1	0.91	0.21	68,68,68,68	0
58	MG	1A	3583	1/1	0.91	0.23	29,29,29,29	0
58	MG	1A	3640	1/1	0.91	0.15	33,33,33,33	0
58	MG	2A	3800	1/1	0.91	0.16	52,52,52,52	0
58	MG	2A	3326	1/1	0.91	0.14	66,66,66,66	0
58	MG	2A	3802	1/1	0.91	0.17	39,39,39,39	0
58	MG	2A	3084	1/1	0.91	0.20	44,44,44,44	0
58	MG	1A	3724	1/1	0.91	0.27	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3726	1/1	0.91	0.34	43,43,43,43	0
58	MG	1A	3584	1/1	0.91	0.23	40,40,40,40	0
58	MG	1A	3585	1/1	0.91	0.11	48,48,48,48	0
58	MG	2A	3811	1/1	0.91	0.17	65,65,65,65	0
58	MG	1A	3645	1/1	0.91	0.22	56,56,56,56	0
58	MG	1A	3932	1/1	0.91	0.14	33,33,33,33	0
58	MG	2a	1817	1/1	0.91	0.11	65,65,65,65	0
58	MG	1A	3835	1/1	0.91	0.10	45,45,45,45	0
58	MG	1a	1676	1/1	0.91	0.10	58,58,58,58	0
58	MG	1A	3371	1/1	0.91	0.20	47,47,47,47	0
58	MG	1A	3839	1/1	0.91	0.12	34,34,34,34	0
58	MG	13	102	1/1	0.91	0.20	37,37,37,37	0
58	MG	2e	201	1/1	0.91	0.16	71,71,71,71	0
58	MG	2A	3341	1/1	0.91	0.14	54,54,54,54	0
58	MG	1A	3655	1/1	0.91	0.15	65,65,65,65	0
58	MG	2A	3230	1/1	0.91	0.30	68,68,68,68	0
58	MG	2a	1656	1/1	0.91	0.11	62,62,62,62	0
58	MG	2A	3647	1/1	0.91	0.15	49,49,49,49	0
58	MG	1A	3663	1/1	0.91	0.15	35,35,35,35	0
58	MG	1A	3322	1/1	0.91	0.32	41,41,41,41	0
58	MG	2A	3829	1/1	0.91	0.19	37,37,37,37	0
58	MG	1A	3239	1/1	0.91	0.25	29,29,29,29	0
58	MG	2t	201	1/1	0.91	0.32	59,59,59,59	0
58	MG	1A	3538	1/1	0.91	0.26	27,27,27,27	0
58	MG	1A	3241	1/1	0.91	0.19	40,40,40,40	0
58	MG	1A	3501	1/1	0.91	0.23	41,41,41,41	0
58	MG	1A	3596	1/1	0.91	0.20	54,54,54,54	0
58	MG	2A	3354	1/1	0.91	0.21	39,39,39,39	0
58	MG	1B	225	1/1	0.91	0.30	52,52,52,52	0
58	MG	1A	3757	1/1	0.91	0.21	47,47,47,47	0
58	MG	1a	1809	1/1	0.91	0.12	39,39,39,39	0
58	MG	1a	1810	1/1	0.91	0.10	55,55,55,55	0
58	MG	1A	3197	1/1	0.91	0.20	36,36,36,36	0
58	MG	2A	3247	1/1	0.91	0.18	60,60,60,60	0
58	MG	2A	3248	1/1	0.91	0.27	48,48,48,48	0
58	MG	2A	3129	1/1	0.91	0.18	41,41,41,41	0
60	ZN	14	102	1/1	0.91	0.05	100,100,100,100	0
58	MG	1d	301	1/1	0.91	0.29	55,55,55,55	0
58	MG	2A	3678	1/1	0.91	0.23	57,57,57,57	0
58	MG	1A	4037	1/1	0.92	0.20	40,40,40,40	0
58	MG	2a	1675	1/1	0.92	0.14	54,54,54,54	0
58	MG	1a	1721	1/1	0.92	0.22	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3634	1/1	0.92	0.22	35,35,35,35	0
58	MG	2a	1678	1/1	0.92	0.22	59,59,59,59	0
58	MG	1A	3656	1/1	0.92	0.15	48,48,48,48	0
58	MG	1A	3845	1/1	0.92	0.16	39,39,39,39	0
58	MG	1A	3659	1/1	0.92	0.26	38,38,38,38	0
58	MG	2A	3453	1/1	0.92	0.23	70,70,70,70	0
58	MG	1a	1613	1/1	0.92	0.09	47,47,47,47	0
58	MG	1A	3440	1/1	0.92	0.15	46,46,46,46	0
58	MG	1A	4044	1/1	0.92	0.28	38,38,38,38	0
58	MG	2A	3026	1/1	0.92	0.25	47,47,47,47	0
58	MG	1A	3079	1/1	0.92	0.21	24,24,24,24	0
58	MG	1A	4046	1/1	0.92	0.10	53,53,53,53	0
58	MG	2A	3188	1/1	0.92	0.16	51,51,51,51	0
58	MG	2A	3033	1/1	0.92	0.17	37,37,37,37	0
58	MG	2A	3846	1/1	0.92	0.09	49,49,49,49	0
58	MG	2A	3034	1/1	0.92	0.14	52,52,52,52	0
58	MG	1a	1738	1/1	0.92	0.22	48,48,48,48	0
58	MG	1a	1739	1/1	0.92	0.10	56,56,56,56	0
58	MG	1A	3177	1/1	0.92	0.24	35,35,35,35	0
58	MG	1A	3243	1/1	0.92	0.18	40,40,40,40	0
58	MG	1A	3747	1/1	0.92	0.28	19,19,19,19	0
58	MG	2a	1703	1/1	0.92	0.15	65,65,65,65	0
58	MG	1A	3223	1/1	0.92	0.16	37,37,37,37	0
58	MG	1A	3754	1/1	0.92	0.16	37,37,37,37	0
58	MG	1A	3365	1/1	0.92	0.20	32,32,32,32	0
58	MG	1A	4054	1/1	0.92	0.22	36,36,36,36	0
58	MG	2A	3051	1/1	0.92	0.17	63,63,63,63	0
58	MG	2A	3052	1/1	0.92	0.33	46,46,46,46	0
58	MG	2B	213	1/1	0.92	0.26	58,58,58,58	0
58	MG	2A	3202	1/1	0.92	0.27	55,55,55,55	0
58	MG	1A	3367	1/1	0.92	0.19	42,42,42,42	0
58	MG	1A	3368	1/1	0.92	0.15	49,49,49,49	0
58	MG	2A	3485	1/1	0.92	0.24	53,53,53,53	0
58	MG	1A	3102	1/1	0.92	0.21	63,63,63,63	0
58	MG	1A	3010	1/1	0.92	0.17	30,30,30,30	0
58	MG	2A	3684	1/1	0.92	0.09	61,61,61,61	0
58	MG	2a	1723	1/1	0.92	0.29	64,64,64,64	0
58	MG	1I	201	1/1	0.92	0.14	55,55,55,55	0
58	MG	2A	3686	1/1	0.92	0.19	46,46,46,46	0
58	MG	2A	3339	1/1	0.92	0.18	74,74,74,74	0
58	MG	2A	3059	1/1	0.92	0.21	51,51,51,51	0
58	MG	1A	3340	1/1	0.92	0.13	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	4062	1/1	0.92	0.21	18,18,18,18	0
58	MG	1A	3967	1/1	0.92	0.23	25,25,25,25	0
58	MG	1A	3968	1/1	0.92	0.09	33,33,33,33	0
58	MG	1P	203	1/1	0.92	0.14	32,32,32,32	0
58	MG	1P	207	1/1	0.92	0.11	34,34,34,34	0
58	MG	2A	3216	1/1	0.92	0.21	52,52,52,52	0
58	MG	2A	3068	1/1	0.92	0.32	51,51,51,51	0
58	MG	1A	3679	1/1	0.92	0.15	23,23,23,23	0
58	MG	1A	3682	1/1	0.92	0.17	27,27,27,27	0
58	MG	1A	3768	1/1	0.92	0.18	27,27,27,27	0
58	MG	2A	3508	1/1	0.92	0.26	38,38,38,38	0
58	MG	1A	3549	1/1	0.92	0.28	59,59,59,59	0
58	MG	1A	3685	1/1	0.92	0.13	58,58,58,58	0
58	MG	2A	3512	1/1	0.92	0.31	50,50,50,50	0
58	MG	2A	3080	1/1	0.92	0.10	45,45,45,45	0
58	MG	2A	3516	1/1	0.92	0.18	43,43,43,43	0
58	MG	1A	3550	1/1	0.92	0.11	33,33,33,33	0
58	MG	1S	202	1/1	0.92	0.21	49,49,49,49	0
58	MG	1A	3372	1/1	0.92	0.16	54,54,54,54	0
58	MG	1A	3057	1/1	0.92	0.18	44,44,44,44	0
58	MG	1a	1775	1/1	0.92	0.10	70,70,70,70	0
58	MG	1U	203	1/1	0.92	0.43	40,40,40,40	0
58	MG	2A	3236	1/1	0.92	0.17	62,62,62,62	0
58	MG	2a	1757	1/1	0.92	0.16	46,46,46,46	0
58	MG	1A	4085	1/1	0.92	0.25	69,69,69,69	0
58	MG	1a	1658	1/1	0.92	0.30	47,47,47,47	0
58	MG	1A	3614	1/1	0.92	0.17	54,54,54,54	0
58	MG	1A	3692	1/1	0.92	0.16	32,32,32,32	0
58	MG	2A	3737	1/1	0.92	0.13	56,56,56,56	0
58	MG	1A	3133	1/1	0.92	0.21	38,38,38,38	0
58	MG	2W	201	1/1	0.92	0.35	61,61,61,61	0
58	MG	1A	3458	1/1	0.92	0.33	51,51,51,51	0
58	MG	1W	201	1/1	0.92	0.44	53,53,53,53	0
58	MG	1A	3377	1/1	0.92	0.27	50,50,50,50	0
58	MG	2A	3104	1/1	0.92	0.09	58,58,58,58	0
58	MG	2A	3542	1/1	0.92	0.13	42,42,42,42	0
58	MG	2A	3544	1/1	0.92	0.16	48,48,48,48	0
58	MG	2A	3105	1/1	0.92	0.15	43,43,43,43	0
58	MG	27	101	1/1	0.92	0.21	45,45,45,45	0
58	MG	1A	4091	1/1	0.92	0.20	44,44,44,44	0
58	MG	1Y	202	1/1	0.92	0.20	51,51,51,51	0
58	MG	1A	3785	1/1	0.92	0.14	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1a	1668	1/1	0.92	0.10	55,55,55,55	0
58	MG	2A	3555	1/1	0.92	0.09	40,40,40,40	0
58	MG	2a	1785	1/1	0.92	0.11	60,60,60,60	0
58	MG	2A	3114	1/1	0.92	0.32	56,56,56,56	0
58	MG	2A	3756	1/1	0.92	0.09	60,60,60,60	0
58	MG	2A	3757	1/1	0.92	0.10	59,59,59,59	0
58	MG	1A	3105	1/1	0.92	0.14	43,43,43,43	0
58	MG	1A	3621	1/1	0.92	0.18	27,27,27,27	0
58	MG	1a	1797	1/1	0.92	0.10	45,45,45,45	0
58	MG	1A	3063	1/1	0.92	0.27	41,41,41,41	0
58	MG	2a	1612	1/1	0.92	0.21	59,59,59,59	0
58	MG	2A	3565	1/1	0.92	0.16	34,34,34,34	0
58	MG	1Z	304	1/1	0.92	0.22	58,58,58,58	0
58	MG	2A	3767	1/1	0.92	0.17	52,52,52,52	0
58	MG	1A	3790	1/1	0.92	0.19	31,31,31,31	0
58	MG	1A	3902	1/1	0.92	0.30	41,41,41,41	0
58	MG	10	106	1/1	0.92	0.17	45,45,45,45	0
58	MG	2A	3771	1/1	0.92	0.20	71,71,71,71	0
58	MG	2A	3400	1/1	0.92	0.37	60,60,60,60	0
58	MG	2A	3401	1/1	0.92	0.23	50,50,50,50	0
58	MG	1A	3903	1/1	0.92	0.10	49,49,49,49	0
58	MG	1A	3345	1/1	0.92	0.25	30,30,30,30	0
58	MG	1a	1681	1/1	0.92	0.20	53,53,53,53	0
58	MG	1A	3907	1/1	0.92	0.16	32,32,32,32	0
58	MG	1A	3427	1/1	0.92	0.25	50,50,50,50	0
58	MG	1A	3706	1/1	0.92	0.20	32,32,32,32	0
58	MG	1A	3383	1/1	0.92	0.21	43,43,43,43	0
58	MG	1A	3570	1/1	0.92	0.18	50,50,50,50	0
58	MG	2A	3785	1/1	0.92	0.09	65,65,65,65	0
58	MG	1B	207	1/1	0.92	0.15	46,46,46,46	0
58	MG	1A	3632	1/1	0.92	0.20	23,23,23,23	0
58	MG	13	101	1/1	0.92	0.22	33,33,33,33	0
58	MG	1A	3917	1/1	0.92	0.22	34,34,34,34	0
58	MG	1A	3168	1/1	0.92	0.13	46,46,46,46	0
58	MG	1A	3271	1/1	0.92	0.19	38,38,38,38	0
58	MG	2d	302	1/1	0.92	0.14	62,62,62,62	0
58	MG	1A	3193	1/1	0.92	0.15	35,35,35,35	0
58	MG	1A	3274	1/1	0.92	0.14	41,41,41,41	0
58	MG	1A	3582	1/1	0.92	0.20	57,57,57,57	0
58	MG	1A	4021	1/1	0.92	0.16	51,51,51,51	0
58	MG	2a	1645	1/1	0.92	0.25	57,57,57,57	0
58	MG	1A	3011	1/1	0.92	0.12	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3393	1/1	0.92	0.14	63,63,63,63	0
58	MG	1A	3326	1/1	0.92	0.17	58,58,58,58	0
58	MG	1A	3357	1/1	0.92	0.19	53,53,53,53	0
58	MG	1a	1705	1/1	0.92	0.10	57,57,57,57	0
58	MG	1A	3818	1/1	0.92	0.13	53,53,53,53	0
58	MG	2A	3605	1/1	0.92	0.22	55,55,55,55	0
58	MG	1A	3725	1/1	0.92	0.13	40,40,40,40	0
58	MG	2A	3164	1/1	0.92	0.28	58,58,58,58	0
58	MG	1A	3832	1/1	0.92	0.23	46,46,46,46	0
58	MG	2A	3810	1/1	0.92	0.13	45,45,45,45	0
58	MG	1A	3649	1/1	0.92	0.07	64,64,64,64	0
58	MG	2A	3434	1/1	0.92	0.29	53,53,53,53	0
58	MG	1A	3727	1/1	0.92	0.17	23,23,23,23	0
58	MG	1A	3651	1/1	0.92	0.15	31,31,31,31	0
58	MG	2x	101	1/1	0.92	0.23	44,44,44,44	0
58	MG	1A	3277	1/1	0.92	0.21	37,37,37,37	0
58	MG	2A	3170	1/1	0.92	0.13	41,41,41,41	0
58	MG	2A	3818	1/1	0.92	0.16	32,32,32,32	0
58	MG	1A	3731	1/1	0.92	0.14	56,56,56,56	0
58	MG	2A	3299	1/1	0.92	0.15	58,58,58,58	0
58	MG	2A	3006	1/1	0.92	0.14	58,58,58,58	0
58	MG	1A	3945	1/1	0.92	0.24	30,30,30,30	0
58	MG	1A	3280	1/1	0.92	0.46	37,37,37,37	0
61	SF4	2d	304	8/8	0.92	0.12	61,70,76,84	0
58	MG	1P	204	1/1	0.93	0.17	29,29,29,29	0
58	MG	1A	3508	1/1	0.93	0.14	41,41,41,41	0
58	MG	2a	1669	1/1	0.93	0.16	35,35,35,35	0
58	MG	1A	3593	1/1	0.93	0.45	40,40,40,40	0
58	MG	1A	3853	1/1	0.93	0.13	55,55,55,55	0
58	MG	1A	4005	1/1	0.93	0.21	26,26,26,26	0
58	MG	1A	3479	1/1	0.93	0.38	49,49,49,49	0
58	MG	1a	1635	1/1	0.93	0.15	49,49,49,49	0
58	MG	2A	3039	1/1	0.93	0.33	55,55,55,55	0
58	MG	2A	3452	1/1	0.93	0.33	50,50,50,50	0
58	MG	2A	3628	1/1	0.93	0.14	37,37,37,37	0
58	MG	1R	201	1/1	0.93	0.20	31,31,31,31	0
58	MG	1R	202	1/1	0.93	0.16	39,39,39,39	0
58	MG	1A	4008	1/1	0.93	0.19	23,23,23,23	0
58	MG	1A	3511	1/1	0.93	0.15	28,28,28,28	0
58	MG	2A	3830	1/1	0.93	0.24	33,33,33,33	0
58	MG	1A	4010	1/1	0.93	0.11	36,36,36,36	0
58	MG	1A	3646	1/1	0.93	0.13	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3048	1/1	0.93	0.12	57,57,57,57	0
58	MG	1A	3938	1/1	0.93	0.20	39,39,39,39	0
58	MG	1A	4098	1/1	0.93	0.12	56,56,56,56	0
58	MG	1A	3075	1/1	0.93	0.14	19,19,19,19	0
58	MG	2A	3323	1/1	0.93	0.08	66,66,66,66	0
58	MG	1A	3940	1/1	0.93	0.17	43,43,43,43	0
58	MG	1A	3941	1/1	0.93	0.16	49,49,49,49	0
58	MG	2A	3651	1/1	0.93	0.11	63,63,63,63	0
58	MG	1a	1759	1/1	0.93	0.08	61,61,61,61	0
58	MG	1a	1649	1/1	0.93	0.08	41,41,41,41	0
58	MG	1a	1763	1/1	0.93	0.08	37,37,37,37	0
58	MG	1V	205	1/1	0.93	0.15	34,34,34,34	0
58	MG	2A	3852	1/1	0.93	0.18	54,54,54,54	0
58	MG	1A	3597	1/1	0.93	0.11	45,45,45,45	0
58	MG	1A	3514	1/1	0.93	0.18	28,28,28,28	0
58	MG	1A	3083	1/1	0.93	0.22	41,41,41,41	0
58	MG	2A	3205	1/1	0.93	0.19	66,66,66,66	0
58	MG	2a	1710	1/1	0.93	0.17	59,59,59,59	0
58	MG	1W	202	1/1	0.93	0.27	41,41,41,41	0
58	MG	1A	3784	1/1	0.93	0.17	35,35,35,35	0
58	MG	2B	207	1/1	0.93	0.06	60,60,60,60	0
58	MG	1A	3868	1/1	0.93	0.19	44,44,44,44	0
58	MG	1a	1772	1/1	0.93	0.30	57,57,57,57	0
58	MG	2A	3338	1/1	0.93	0.25	59,59,59,59	0
58	MG	1A	3087	1/1	0.93	0.17	32,32,32,32	0
58	MG	1A	3312	1/1	0.93	0.12	43,43,43,43	0
58	MG	2A	3073	1/1	0.93	0.22	38,38,38,38	0
58	MG	1A	3662	1/1	0.93	0.15	45,45,45,45	0
58	MG	1A	3048	1/1	0.93	0.19	36,36,36,36	0
58	MG	2A	3681	1/1	0.93	0.20	47,47,47,47	0
58	MG	1A	3225	1/1	0.93	0.22	44,44,44,44	0
58	MG	2B	219	1/1	0.93	0.17	54,54,54,54	0
58	MG	1A	3459	1/1	0.93	0.21	56,56,56,56	0
58	MG	1A	3332	1/1	0.93	0.32	55,55,55,55	0
58	MG	2A	3219	1/1	0.93	0.14	44,44,44,44	0
58	MG	2D	306	1/1	0.93	0.18	40,40,40,40	0
58	MG	1a	1780	1/1	0.93	0.12	47,47,47,47	0
58	MG	1A	3491	1/1	0.93	0.18	43,43,43,43	0
58	MG	2A	3085	1/1	0.93	0.12	51,51,51,51	0
58	MG	2A	3691	1/1	0.93	0.16	62,62,62,62	0
58	MG	2A	3503	1/1	0.93	0.56	53,53,53,53	0
58	MG	1A	3209	1/1	0.93	0.19	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	3694	1/1	0.93	0.14	30,30,30,30	0
58	MG	1A	3564	1/1	0.93	0.22	53,53,53,53	0
58	MG	1B	218	1/1	0.93	0.17	45,45,45,45	0
58	MG	2A	3507	1/1	0.93	0.18	49,49,49,49	0
58	MG	1A	3613	1/1	0.93	0.20	25,25,25,25	0
58	MG	2A	3509	1/1	0.93	0.29	66,66,66,66	0
58	MG	1a	1672	1/1	0.93	0.10	50,50,50,50	0
58	MG	2A	3705	1/1	0.93	0.12	52,52,52,52	0
58	MG	2A	3361	1/1	0.93	0.26	45,45,45,45	0
58	MG	1A	3959	1/1	0.93	0.20	55,55,55,55	0
58	MG	2O	201	1/1	0.93	0.15	59,59,59,59	0
58	MG	2A	3363	1/1	0.93	0.17	61,61,61,61	0
58	MG	2A	3515	1/1	0.93	0.18	39,39,39,39	0
58	MG	1a	1674	1/1	0.93	0.20	55,55,55,55	0
58	MG	1A	3733	1/1	0.93	0.18	68,68,68,68	0
58	MG	1l	103	1/1	0.93	0.20	41,41,41,41	0
58	MG	2A	3235	1/1	0.93	0.21	54,54,54,54	0
58	MG	2Q	204	1/1	0.93	0.14	42,42,42,42	0
58	MG	2A	3719	1/1	0.93	0.13	43,43,43,43	0
58	MG	1A	4039	1/1	0.93	0.16	46,46,46,46	0
58	MG	2a	1763	1/1	0.93	0.23	59,59,59,59	0
58	MG	1l	105	1/1	0.93	0.12	63,63,63,63	0
58	MG	2A	3522	1/1	0.93	0.13	61,61,61,61	0
58	MG	1A	3565	1/1	0.93	0.26	35,35,35,35	0
58	MG	1B	227	1/1	0.93	0.26	46,46,46,46	0
58	MG	1A	3889	1/1	0.93	0.21	28,28,28,28	0
58	MG	2A	3527	1/1	0.93	0.06	29,29,29,29	0
58	MG	2A	3729	1/1	0.93	0.08	60,60,60,60	0
58	MG	1A	3398	1/1	0.93	0.15	29,29,29,29	0
58	MG	2A	3530	1/1	0.93	0.12	32,32,32,32	0
58	MG	2A	3734	1/1	0.93	0.28	50,50,50,50	0
58	MG	1a	1684	1/1	0.93	0.25	67,67,67,67	0
58	MG	2a	1777	1/1	0.93	0.14	53,53,53,53	0
58	MG	1A	3965	1/1	0.93	0.10	31,31,31,31	0
58	MG	2A	3113	1/1	0.93	0.22	50,50,50,50	0
58	MG	2a	1780	1/1	0.93	0.17	67,67,67,67	0
58	MG	2A	3739	1/1	0.93	0.12	43,43,43,43	0
58	MG	1A	3528	1/1	0.93	0.22	41,41,41,41	0
58	MG	1a	1806	1/1	0.93	0.12	54,54,54,54	0
58	MG	2A	3537	1/1	0.93	0.19	38,38,38,38	0
58	MG	1A	3228	1/1	0.93	0.19	28,28,28,28	0
58	MG	1A	3619	1/1	0.93	0.15	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3496	1/1	0.93	0.17	26,26,26,26	0
58	MG	2A	3543	1/1	0.93	0.11	38,38,38,38	0
58	MG	29	101	1/1	0.93	0.26	61,61,61,61	0
58	MG	1A	3745	1/1	0.93	0.20	57,57,57,57	0
58	MG	1A	3972	1/1	0.93	0.07	53,53,53,53	0
58	MG	1A	3572	1/1	0.93	0.19	31,31,31,31	0
58	MG	1A	3900	1/1	0.93	0.20	66,66,66,66	0
58	MG	1A	3576	1/1	0.93	0.18	49,49,49,49	0
58	MG	2a	1797	1/1	0.93	0.17	47,47,47,47	0
58	MG	2A	3390	1/1	0.93	0.21	43,43,43,43	0
58	MG	2a	1607	1/1	0.93	0.16	56,56,56,56	0
58	MG	1E	302	1/1	0.93	0.16	36,36,36,36	0
58	MG	18	104	1/1	0.93	0.27	41,41,41,41	0
58	MG	2A	3393	1/1	0.93	0.23	39,39,39,39	0
58	MG	1l	202	1/1	0.93	0.08	58,58,58,58	0
58	MG	1m	3001	1/1	0.93	0.07	51,51,51,51	0
58	MG	1E	304	1/1	0.93	0.14	33,33,33,33	0
58	MG	1E	305	1/1	0.93	0.39	54,54,54,54	0
58	MG	1w	101	1/1	0.93	0.19	66,66,66,66	0
58	MG	2A	3763	1/1	0.93	0.17	41,41,41,41	0
58	MG	2A	3567	1/1	0.93	0.13	49,49,49,49	0
58	MG	1A	3819	1/1	0.93	0.21	63,63,63,63	0
58	MG	1A	3904	1/1	0.93	0.14	33,33,33,33	0
58	MG	1a	1702	1/1	0.93	0.13	51,51,51,51	0
58	MG	2A	3142	1/1	0.93	0.10	46,46,46,46	0
58	MG	1A	3532	1/1	0.93	0.19	55,55,55,55	0
58	MG	1A	3830	1/1	0.93	0.16	34,34,34,34	0
58	MG	2A	3574	1/1	0.93	0.18	35,35,35,35	0
58	MG	2A	3271	1/1	0.93	0.19	60,60,60,60	0
58	MG	2A	3775	1/1	0.93	0.11	54,54,54,54	0
58	MG	2A	3145	1/1	0.93	0.14	50,50,50,50	0
58	MG	2A	3412	1/1	0.93	0.12	49,49,49,49	0
58	MG	1A	3627	1/1	0.93	0.23	29,29,29,29	0
58	MG	1A	3419	1/1	0.93	0.23	49,49,49,49	0
58	MG	2f	201	1/1	0.93	0.15	42,42,42,42	0
58	MG	2A	3149	1/1	0.93	0.17	43,43,43,43	0
58	MG	1A	4065	1/1	0.93	0.19	58,58,58,58	0
58	MG	1A	3983	1/1	0.93	0.34	53,53,53,53	0
58	MG	2A	3586	1/1	0.93	0.09	58,58,58,58	0
58	MG	1A	3837	1/1	0.93	0.14	50,50,50,50	0
58	MG	2A	3588	1/1	0.93	0.26	53,53,53,53	0
58	MG	1A	3691	1/1	0.93	0.22	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3499	1/1	0.93	0.18	33,33,33,33	0
58	MG	1A	3211	1/1	0.93	0.12	39,39,39,39	0
58	MG	2r	101	1/1	0.93	0.19	63,63,63,63	0
58	MG	1A	3014	1/1	0.93	0.24	26,26,26,26	0
58	MG	2A	3159	1/1	0.93	0.13	55,55,55,55	0
58	MG	1a	1718	1/1	0.93	0.10	66,66,66,66	0
58	MG	1A	3081	1/1	0.93	0.18	36,36,36,36	0
58	MG	2A	3795	1/1	0.93	0.13	41,41,41,41	0
58	MG	1G	204	1/1	0.93	0.12	59,59,59,59	0
58	MG	2A	3163	1/1	0.93	0.09	54,54,54,54	0
58	MG	1a	1618	1/1	0.93	0.17	53,53,53,53	0
58	MG	1a	1723	1/1	0.93	0.24	50,50,50,50	0
58	MG	2w	104	1/1	0.93	0.10	70,70,70,70	0
58	MG	1A	4078	1/1	0.93	0.32	34,34,34,34	0
58	MG	2A	3010	1/1	0.93	0.09	43,43,43,43	0
58	MG	1A	4079	1/1	0.93	0.23	37,37,37,37	0
58	MG	1A	3182	1/1	0.93	0.10	72,72,72,72	0
58	MG	1N	204	1/1	0.93	0.20	48,48,48,48	0
58	MG	1A	3447	1/1	0.93	0.21	38,38,38,38	0
58	MG	1O	203	1/1	0.93	0.25	57,57,57,57	0
60	ZN	1n	103	1/1	0.93	0.09	51,51,51,51	0
58	MG	1A	3170	1/1	0.93	0.20	39,39,39,39	0
58	MG	1A	3288	1/1	0.93	0.16	38,38,38,38	0
58	MG	1A	3849	1/1	0.93	0.15	57,57,57,57	0
58	MG	2A	3352	1/1	0.94	0.51	65,65,65,65	0
58	MG	1U	205	1/1	0.94	0.22	33,33,33,33	0
58	MG	1A	4068	1/1	0.94	0.17	44,44,44,44	0
58	MG	1U	208	1/1	0.94	0.23	29,29,29,29	0
58	MG	1A	3381	1/1	0.94	0.13	36,36,36,36	0
58	MG	1A	3554	1/1	0.94	0.21	29,29,29,29	0
58	MG	1A	3112	1/1	0.94	0.16	29,29,29,29	0
58	MG	1A	3188	1/1	0.94	0.16	30,30,30,30	0
58	MG	1A	3557	1/1	0.94	0.32	39,39,39,39	0
58	MG	2A	3546	1/1	0.94	0.14	38,38,38,38	0
58	MG	2A	3547	1/1	0.94	0.12	46,46,46,46	0
58	MG	1A	3492	1/1	0.94	0.15	42,42,42,42	0
58	MG	1A	3189	1/1	0.94	0.18	34,34,34,34	0
58	MG	1A	3190	1/1	0.94	0.14	43,43,43,43	0
58	MG	2A	3552	1/1	0.94	0.11	39,39,39,39	0
58	MG	1A	3638	1/1	0.94	0.18	25,25,25,25	0
58	MG	1A	3386	1/1	0.94	0.22	38,38,38,38	0
58	MG	2a	1657	1/1	0.94	0.10	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3847	1/1	0.94	0.20	30,30,30,30	0
58	MG	1A	4083	1/1	0.94	0.20	50,50,50,50	0
58	MG	2A	3028	1/1	0.94	0.13	38,38,38,38	0
58	MG	1A	4084	1/1	0.94	0.20	45,45,45,45	0
58	MG	2A	3562	1/1	0.94	0.18	38,38,38,38	0
58	MG	2A	3031	1/1	0.94	0.23	38,38,38,38	0
58	MG	2A	3564	1/1	0.94	0.14	40,40,40,40	0
58	MG	1a	1703	1/1	0.94	0.25	49,49,49,49	0
58	MG	2a	1666	1/1	0.94	0.17	58,58,58,58	0
58	MG	1A	3113	1/1	0.94	0.15	28,28,28,28	0
58	MG	1A	3732	1/1	0.94	0.12	42,42,42,42	0
58	MG	1A	3641	1/1	0.94	0.14	19,19,19,19	0
58	MG	1a	1707	1/1	0.94	0.12	41,41,41,41	0
58	MG	1A	3736	1/1	0.94	0.15	22,22,22,22	0
58	MG	1A	3642	1/1	0.94	0.08	49,49,49,49	0
58	MG	1A	3230	1/1	0.94	0.17	44,44,44,44	0
58	MG	1A	3855	1/1	0.94	0.12	49,49,49,49	0
58	MG	1A	3306	1/1	0.94	0.17	30,30,30,30	0
58	MG	1A	3114	1/1	0.94	0.18	28,28,28,28	0
58	MG	1A	3041	1/1	0.94	0.13	33,33,33,33	0
58	MG	1A	3863	1/1	0.94	0.18	37,37,37,37	0
58	MG	2A	3578	1/1	0.94	0.18	30,30,30,30	0
58	MG	1A	3975	1/1	0.94	0.10	56,56,56,56	0
58	MG	1A	3267	1/1	0.94	0.39	45,45,45,45	0
58	MG	1A	3349	1/1	0.94	0.21	38,38,38,38	0
58	MG	1A	3086	1/1	0.94	0.32	28,28,28,28	0
58	MG	1A	3052	1/1	0.94	0.21	24,24,24,24	0
58	MG	1A	3748	1/1	0.94	0.17	24,24,24,24	0
58	MG	2A	3057	1/1	0.94	0.14	40,40,40,40	0
58	MG	1A	3749	1/1	0.94	0.19	22,22,22,22	0
58	MG	2A	3399	1/1	0.94	0.39	51,51,51,51	0
58	MG	1A	3448	1/1	0.94	0.17	55,55,55,55	0
58	MG	1B	204	1/1	0.94	0.34	59,59,59,59	0
58	MG	2A	3402	1/1	0.94	0.16	36,36,36,36	0
58	MG	1a	1730	1/1	0.94	0.14	39,39,39,39	0
58	MG	2A	3595	1/1	0.94	0.13	53,53,53,53	0
58	MG	15	101	1/1	0.94	0.23	27,27,27,27	0
58	MG	1A	3658	1/1	0.94	0.11	37,37,37,37	0
58	MG	1A	3449	1/1	0.94	0.20	42,42,42,42	0
58	MG	15	106	1/1	0.94	0.18	50,50,50,50	0
58	MG	15	107	1/1	0.94	0.17	54,54,54,54	0
58	MG	2a	1707	1/1	0.94	0.15	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3660	1/1	0.94	0.24	45,45,45,45	0
58	MG	17	104	1/1	0.94	0.15	49,49,49,49	0
58	MG	1A	3876	1/1	0.94	0.12	39,39,39,39	0
58	MG	2A	3074	1/1	0.94	0.12	40,40,40,40	0
58	MG	1A	3988	1/1	0.94	0.17	30,30,30,30	0
58	MG	2A	3828	1/1	0.94	0.13	49,49,49,49	0
58	MG	1B	210	1/1	0.94	0.40	52,52,52,52	0
58	MG	1A	3174	1/1	0.94	0.16	27,27,27,27	0
58	MG	2A	3831	1/1	0.94	0.04	55,55,55,55	0
58	MG	1A	3238	1/1	0.94	0.14	31,31,31,31	0
58	MG	2a	1719	1/1	0.94	0.12	68,68,68,68	0
58	MG	1A	3120	1/1	0.94	0.20	44,44,44,44	0
58	MG	1A	3993	1/1	0.94	0.20	45,45,45,45	0
58	MG	2A	3083	1/1	0.94	0.29	53,53,53,53	0
58	MG	1A	3994	1/1	0.94	0.09	36,36,36,36	0
58	MG	1A	3667	1/1	0.94	0.16	20,20,20,20	0
58	MG	1A	3513	1/1	0.94	0.22	30,30,30,30	0
58	MG	1A	3997	1/1	0.94	0.16	10,10,10,10	0
58	MG	2a	1728	1/1	0.94	0.21	69,69,69,69	0
58	MG	1A	3763	1/1	0.94	0.19	27,27,27,27	0
58	MG	2A	3842	1/1	0.94	0.12	49,49,49,49	0
58	MG	1A	3273	1/1	0.94	0.13	27,27,27,27	0
58	MG	1A	3515	1/1	0.94	0.14	33,33,33,33	0
58	MG	2A	3261	1/1	0.94	0.19	57,57,57,57	0
58	MG	2A	3847	1/1	0.94	0.20	61,61,61,61	0
58	MG	1A	3317	1/1	0.94	0.35	54,54,54,54	0
58	MG	1A	3240	1/1	0.94	0.29	32,32,32,32	0
58	MG	2A	3629	1/1	0.94	0.18	41,41,41,41	0
58	MG	2A	3098	1/1	0.94	0.12	26,26,26,26	0
58	MG	2A	3633	1/1	0.94	0.09	46,46,46,46	0
58	MG	1B	226	1/1	0.94	0.20	62,62,62,62	0
58	MG	2A	3635	1/1	0.94	0.19	41,41,41,41	0
58	MG	1A	3892	1/1	0.94	0.12	28,28,28,28	0
58	MG	2A	3101	1/1	0.94	0.13	44,44,44,44	0
58	MG	2A	3638	1/1	0.94	0.22	40,40,40,40	0
58	MG	1a	1762	1/1	0.94	0.09	71,71,71,71	0
58	MG	2B	209	1/1	0.94	0.06	58,58,58,58	0
58	MG	1A	3148	1/1	0.94	0.49	42,42,42,42	0
58	MG	1A	4006	1/1	0.94	0.08	27,27,27,27	0
58	MG	1A	3101	1/1	0.94	0.16	40,40,40,40	0
58	MG	2A	3106	1/1	0.94	0.11	56,56,56,56	0
58	MG	1a	1616	1/1	0.94	0.10	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	3646	1/1	0.94	0.21	47,47,47,47	0
58	MG	1A	3208	1/1	0.94	0.17	37,37,37,37	0
58	MG	1A	3178	1/1	0.94	0.27	36,36,36,36	0
58	MG	2A	3111	1/1	0.94	0.24	49,49,49,49	0
58	MG	1A	3012	1/1	0.94	0.13	26,26,26,26	0
58	MG	1A	3070	1/1	0.94	0.24	22,22,22,22	0
58	MG	1B	237	1/1	0.94	0.12	40,40,40,40	0
58	MG	1B	238	1/1	0.94	0.14	29,29,29,29	0
58	MG	1D	302	1/1	0.94	0.22	46,46,46,46	0
58	MG	2A	3656	1/1	0.94	0.21	58,58,58,58	0
58	MG	2A	3117	1/1	0.94	0.12	53,53,53,53	0
58	MG	2A	3659	1/1	0.94	0.13	55,55,55,55	0
58	MG	2A	3454	1/1	0.94	0.14	47,47,47,47	0
58	MG	1A	4012	1/1	0.94	0.17	34,34,34,34	0
58	MG	1D	304	1/1	0.94	0.25	43,43,43,43	0
58	MG	1D	305	1/1	0.94	0.12	36,36,36,36	0
58	MG	2A	3669	1/1	0.94	0.15	58,58,58,58	0
58	MG	2A	3460	1/1	0.94	0.16	62,62,62,62	0
58	MG	1A	4013	1/1	0.94	0.16	53,53,53,53	0
58	MG	1A	3414	1/1	0.94	0.19	43,43,43,43	0
58	MG	2A	3124	1/1	0.94	0.13	65,65,65,65	0
58	MG	1A	4016	1/1	0.94	0.08	64,64,64,64	0
58	MG	1A	3464	1/1	0.94	0.20	38,38,38,38	0
58	MG	1A	3249	1/1	0.94	0.17	28,28,28,28	0
58	MG	2A	3468	1/1	0.94	0.17	56,56,56,56	0
58	MG	1a	1632	1/1	0.94	0.22	24,24,24,24	0
58	MG	1A	3467	1/1	0.94	0.19	37,37,37,37	0
58	MG	1A	3905	1/1	0.94	0.14	37,37,37,37	0
58	MG	1E	307	1/1	0.94	0.14	50,50,50,50	0
58	MG	2A	3473	1/1	0.94	0.08	34,34,34,34	0
58	MG	1a	1790	1/1	0.94	0.11	45,45,45,45	0
58	MG	1A	3468	1/1	0.94	0.10	38,38,38,38	0
58	MG	1A	3787	1/1	0.94	0.19	28,28,28,28	0
58	MG	2a	1792	1/1	0.94	0.12	63,63,63,63	0
58	MG	1A	3046	1/1	0.94	0.33	26,26,26,26	0
58	MG	1A	3470	1/1	0.94	0.38	50,50,50,50	0
58	MG	1A	3013	1/1	0.94	0.20	23,23,23,23	0
58	MG	1A	3418	1/1	0.94	0.22	52,52,52,52	0
58	MG	2A	3305	1/1	0.94	0.17	59,59,59,59	0
58	MG	1A	3093	1/1	0.94	0.18	22,22,22,22	0
58	MG	2A	3696	1/1	0.94	0.20	59,59,59,59	0
58	MG	1F	307	1/1	0.94	0.20	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3914	1/1	0.94	0.21	34,34,34,34	0
58	MG	1A	3915	1/1	0.94	0.17	34,34,34,34	0
58	MG	2A	3700	1/1	0.94	0.23	31,31,31,31	0
58	MG	1A	3916	1/1	0.94	0.14	32,32,32,32	0
58	MG	2X	3500	1/1	0.94	0.09	52,52,52,52	0
58	MG	1A	3795	1/1	0.94	0.19	68,68,68,68	0
58	MG	2Z	301	1/1	0.94	0.14	68,68,68,68	0
58	MG	2A	3704	1/1	0.94	0.14	43,43,43,43	0
58	MG	1A	3420	1/1	0.94	0.33	61,61,61,61	0
58	MG	2A	3152	1/1	0.94	0.17	42,42,42,42	0
58	MG	2A	3707	1/1	0.94	0.13	61,61,61,61	0
58	MG	2A	3708	1/1	0.94	0.09	49,49,49,49	0
58	MG	1A	3540	1/1	0.94	0.12	47,47,47,47	0
58	MG	1a	1653	1/1	0.94	0.19	41,41,41,41	0
58	MG	1A	3799	1/1	0.94	0.21	18,18,18,18	0
58	MG	1A	3923	1/1	0.94	0.15	35,35,35,35	0
58	MG	28	103	1/1	0.94	0.20	60,60,60,60	0
58	MG	1G	205	1/1	0.94	0.16	61,61,61,61	0
58	MG	1A	3800	1/1	0.94	0.25	17,17,17,17	0
58	MG	2A	3500	1/1	0.94	0.21	68,68,68,68	0
58	MG	1A	3925	1/1	0.94	0.09	35,35,35,35	0
58	MG	1A	3018	1/1	0.94	0.23	27,27,27,27	0
58	MG	1A	3699	1/1	0.94	0.25	23,23,23,23	0
58	MG	1N	205	1/1	0.94	0.30	45,45,45,45	0
58	MG	1A	3330	1/1	0.94	0.16	43,43,43,43	0
58	MG	1A	3702	1/1	0.94	0.14	33,33,33,33	0
58	MG	1A	3424	1/1	0.94	0.22	30,30,30,30	0
58	MG	1A	3425	1/1	0.94	0.15	37,37,37,37	0
58	MG	2a	1610	1/1	0.94	0.19	52,52,52,52	0
58	MG	1A	3331	1/1	0.94	0.13	42,42,42,42	0
58	MG	1A	3934	1/1	0.94	0.15	11,11,11,11	0
58	MG	2A	3732	1/1	0.94	0.25	35,35,35,35	0
58	MG	1w	102	1/1	0.94	0.18	46,46,46,46	0
58	MG	1P	206	1/1	0.94	0.19	46,46,46,46	0
58	MG	1A	3375	1/1	0.94	0.20	38,38,38,38	0
58	MG	1A	3814	1/1	0.94	0.25	38,38,38,38	0
58	MG	1A	3484	1/1	0.94	0.13	39,39,39,39	0
58	MG	1A	3710	1/1	0.94	0.25	30,30,30,30	0
58	MG	1A	3111	1/1	0.94	0.18	36,36,36,36	0
58	MG	1A	3625	1/1	0.94	0.16	59,59,59,59	0
58	MG	1A	3222	1/1	0.94	0.40	54,54,54,54	0
58	MG	1A	3821	1/1	0.94	0.11	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3715	1/1	0.94	0.13	46,46,46,46	0
58	MG	2A	3745	1/1	0.94	0.24	67,67,67,67	0
58	MG	1S	201	1/1	0.94	0.39	38,38,38,38	0
58	MG	2A	3344	1/1	0.94	0.30	62,62,62,62	0
58	MG	1A	3824	1/1	0.94	0.16	39,39,39,39	0
58	MG	1A	3827	1/1	0.94	0.15	20,20,20,20	0
58	MG	2x	106	1/1	0.94	0.15	51,51,51,51	0
58	MG	2A	3528	1/1	0.94	0.32	63,63,63,63	0
58	MG	1A	3829	1/1	0.94	0.19	39,39,39,39	0
58	MG	1A	3186	1/1	0.94	0.10	40,40,40,40	0
60	ZN	2Y	202	1/1	0.94	0.11	85,85,85,85	0
58	MG	2A	3003	1/1	0.94	0.32	56,56,56,56	0
60	ZN	29	102	1/1	0.94	0.10	57,57,57,57	0
58	MG	1A	3628	1/1	0.94	0.20	26,26,26,26	0
58	MG	2A	3351	1/1	0.94	0.32	54,54,54,54	0
58	MG	1A	3648	1/1	0.95	0.24	47,47,47,47	0
58	MG	2A	3185	1/1	0.95	0.30	49,49,49,49	0
58	MG	2A	3728	1/1	0.95	0.24	49,49,49,49	0
58	MG	1A	3095	1/1	0.95	0.16	52,52,52,52	0
58	MG	1A	3426	1/1	0.95	0.17	38,38,38,38	0
58	MG	2a	1705	1/1	0.95	0.29	65,65,65,65	0
58	MG	2E	307	1/1	0.95	0.11	33,33,33,33	0
58	MG	1A	3878	1/1	0.95	0.17	32,32,32,32	0
58	MG	1a	1785	1/1	0.95	0.11	59,59,59,59	0
58	MG	2A	3066	1/1	0.95	0.17	33,33,33,33	0
58	MG	1A	3879	1/1	0.95	0.20	30,30,30,30	0
58	MG	2A	3444	1/1	0.95	0.23	25,25,25,25	0
58	MG	1a	1787	1/1	0.95	0.17	49,49,49,49	0
58	MG	1A	3880	1/1	0.95	0.16	38,38,38,38	0
58	MG	1A	3150	1/1	0.95	0.12	27,27,27,27	0
58	MG	2A	3072	1/1	0.95	0.29	40,40,40,40	0
58	MG	1A	3964	1/1	0.95	0.23	57,57,57,57	0
58	MG	1A	3007	1/1	0.95	0.11	26,26,26,26	0
58	MG	1D	310	1/1	0.95	0.26	49,49,49,49	0
58	MG	1A	3396	1/1	0.95	0.18	35,35,35,35	0
58	MG	2A	3592	1/1	0.95	0.15	45,45,45,45	0
58	MG	2A	3078	1/1	0.95	0.11	40,40,40,40	0
58	MG	1A	3657	1/1	0.95	0.17	28,28,28,28	0
58	MG	1A	3336	1/1	0.95	0.29	53,53,53,53	0
58	MG	1A	4055	1/1	0.95	0.15	49,49,49,49	0
58	MG	1A	3020	1/1	0.95	0.26	46,46,46,46	0
58	MG	2A	3459	1/1	0.95	0.33	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3366	1/1	0.95	0.20	27,27,27,27	0
58	MG	2a	1730	1/1	0.95	0.24	55,55,55,55	0
58	MG	1A	3971	1/1	0.95	0.15	65,65,65,65	0
58	MG	1A	3507	1/1	0.95	0.12	22,22,22,22	0
58	MG	1A	3029	1/1	0.95	0.20	30,30,30,30	0
58	MG	2A	3087	1/1	0.95	0.19	40,40,40,40	0
58	MG	1A	3891	1/1	0.95	0.22	25,25,25,25	0
58	MG	2A	3089	1/1	0.95	0.24	40,40,40,40	0
58	MG	2A	3606	1/1	0.95	0.20	56,56,56,56	0
58	MG	2A	3090	1/1	0.95	0.22	42,42,42,42	0
58	MG	1A	3664	1/1	0.95	0.30	29,29,29,29	0
58	MG	1A	3434	1/1	0.95	0.25	31,31,31,31	0
58	MG	1A	3339	1/1	0.95	0.21	65,65,65,65	0
58	MG	2A	3095	1/1	0.95	0.21	64,64,64,64	0
58	MG	2A	3217	1/1	0.95	0.21	36,36,36,36	0
58	MG	20	102	1/1	0.95	0.08	50,50,50,50	0
58	MG	2A	3614	1/1	0.95	0.22	52,52,52,52	0
58	MG	1A	3609	1/1	0.95	0.15	34,34,34,34	0
58	MG	23	103	1/1	0.95	0.10	43,43,43,43	0
58	MG	2A	3616	1/1	0.95	0.09	54,54,54,54	0
58	MG	1A	3809	1/1	0.95	0.18	21,21,21,21	0
58	MG	2A	3220	1/1	0.95	0.24	44,44,44,44	0
58	MG	1A	3294	1/1	0.95	0.29	47,47,47,47	0
58	MG	1A	4073	1/1	0.95	0.19	45,45,45,45	0
58	MG	1A	3030	1/1	0.95	0.17	31,31,31,31	0
58	MG	1A	3899	1/1	0.95	0.14	20,20,20,20	0
58	MG	2a	1756	1/1	0.95	0.25	58,58,58,58	0
58	MG	2A	3780	1/1	0.95	0.13	39,39,39,39	0
58	MG	1A	3813	1/1	0.95	0.17	56,56,56,56	0
58	MG	1A	3901	1/1	0.95	0.09	35,35,35,35	0
58	MG	1A	3737	1/1	0.95	0.23	20,20,20,20	0
58	MG	2a	1761	1/1	0.95	0.13	48,48,48,48	0
58	MG	1A	3032	1/1	0.95	0.16	31,31,31,31	0
58	MG	2A	3631	1/1	0.95	0.13	34,34,34,34	0
58	MG	1A	3157	1/1	0.95	0.21	33,33,33,33	0
58	MG	1a	1608	1/1	0.95	0.11	43,43,43,43	0
58	MG	1A	3244	1/1	0.95	0.33	62,62,62,62	0
58	MG	1A	3741	1/1	0.95	0.17	51,51,51,51	0
58	MG	1A	3617	1/1	0.95	0.09	32,32,32,32	0
58	MG	1N	203	1/1	0.95	0.28	47,47,47,47	0
58	MG	1w	106	1/1	0.95	0.65	71,71,71,71	0
58	MG	1A	3276	1/1	0.95	0.09	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	1773	1/1	0.95	0.12	50,50,50,50	0
58	MG	2a	1613	1/1	0.95	0.21	62,62,62,62	0
58	MG	1A	3518	1/1	0.95	0.41	40,40,40,40	0
58	MG	1A	3125	1/1	0.95	0.16	25,25,25,25	0
58	MG	1A	3681	1/1	0.95	0.16	23,23,23,23	0
58	MG	1A	3828	1/1	0.95	0.23	29,29,29,29	0
58	MG	2a	1618	1/1	0.95	0.16	73,73,73,73	0
58	MG	1A	3376	1/1	0.95	0.21	31,31,31,31	0
58	MG	1A	3683	1/1	0.95	0.15	31,31,31,31	0
58	MG	2A	3369	1/1	0.95	0.12	58,58,58,58	0
58	MG	1x	107	1/1	0.95	0.12	47,47,47,47	0
58	MG	2A	3122	1/1	0.95	0.15	39,39,39,39	0
58	MG	2A	3372	1/1	0.95	0.23	38,38,38,38	0
58	MG	1a	1722	1/1	0.95	0.34	55,55,55,55	0
58	MG	1A	3622	1/1	0.95	0.15	10,10,10,10	0
58	MG	1A	4093	1/1	0.95	0.20	54,54,54,54	0
58	MG	2A	3126	1/1	0.95	0.09	40,40,40,40	0
58	MG	2A	3127	1/1	0.95	0.20	44,44,44,44	0
58	MG	2A	3812	1/1	0.95	0.20	54,54,54,54	0
58	MG	2a	1632	1/1	0.95	0.17	51,51,51,51	0
58	MG	1A	3567	1/1	0.95	0.25	23,23,23,23	0
58	MG	1A	3836	1/1	0.95	0.17	56,56,56,56	0
58	MG	1A	3481	1/1	0.95	0.12	36,36,36,36	0
58	MG	1A	3920	1/1	0.95	0.14	37,37,37,37	0
58	MG	2a	1798	1/1	0.95	0.24	53,53,53,53	0
58	MG	2A	3663	1/1	0.95	0.11	39,39,39,39	0
58	MG	1A	3348	1/1	0.95	0.21	29,29,29,29	0
58	MG	2A	3666	1/1	0.95	0.23	36,36,36,36	0
58	MG	1A	3688	1/1	0.95	0.14	18,18,18,18	0
58	MG	1A	3412	1/1	0.95	0.18	37,37,37,37	0
58	MG	1A	3303	1/1	0.95	0.15	22,22,22,22	0
58	MG	1A	3350	1/1	0.95	0.25	59,59,59,59	0
58	MG	2A	3008	1/1	0.95	0.13	36,36,36,36	0
58	MG	2A	3523	1/1	0.95	0.14	36,36,36,36	0
58	MG	1A	3573	1/1	0.95	0.13	35,35,35,35	0
58	MG	1A	3693	1/1	0.95	0.09	30,30,30,30	0
58	MG	1A	3526	1/1	0.95	0.17	42,42,42,42	0
58	MG	2A	3013	1/1	0.95	0.19	35,35,35,35	0
58	MG	1U	201	1/1	0.95	0.21	30,30,30,30	0
58	MG	1A	3764	1/1	0.95	0.15	43,43,43,43	0
58	MG	1A	3051	1/1	0.95	0.21	22,22,22,22	0
58	MG	1A	3766	1/1	0.95	0.23	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3850	1/1	0.95	0.13	45,45,45,45	0
58	MG	2A	3020	1/1	0.95	0.17	36,36,36,36	0
58	MG	1a	1641	1/1	0.95	0.10	51,51,51,51	0
58	MG	1A	3281	1/1	0.95	0.40	31,31,31,31	0
58	MG	2A	3277	1/1	0.95	0.11	63,63,63,63	0
58	MG	1U	207	1/1	0.95	0.15	31,31,31,31	0
58	MG	1A	3282	1/1	0.95	0.17	28,28,28,28	0
58	MG	1A	3530	1/1	0.95	0.28	48,48,48,48	0
58	MG	1A	3636	1/1	0.95	0.12	22,22,22,22	0
58	MG	2i	201	1/1	0.95	0.16	61,61,61,61	0
58	MG	1A	3307	1/1	0.95	0.21	31,31,31,31	0
58	MG	2j	202	1/1	0.95	0.13	61,61,61,61	0
58	MG	1A	3856	1/1	0.95	0.20	20,20,20,20	0
58	MG	1A	3773	1/1	0.95	0.17	36,36,36,36	0
58	MG	2A	3850	1/1	0.95	0.16	46,46,46,46	0
58	MG	1A	3490	1/1	0.95	0.18	27,27,27,27	0
58	MG	2a	1668	1/1	0.95	0.05	61,61,61,61	0
58	MG	1A	3859	1/1	0.95	0.18	23,23,23,23	0
58	MG	1X	102	1/1	0.95	0.17	46,46,46,46	0
58	MG	1a	1655	1/1	0.95	0.19	55,55,55,55	0
58	MG	1X	104	1/1	0.95	0.23	46,46,46,46	0
58	MG	1A	3533	1/1	0.95	0.28	43,43,43,43	0
58	MG	1A	3704	1/1	0.95	0.21	21,21,21,21	0
58	MG	1A	3779	1/1	0.95	0.09	37,37,37,37	0
58	MG	2A	3557	1/1	0.95	0.20	52,52,52,52	0
58	MG	1A	3948	1/1	0.95	0.14	56,56,56,56	0
58	MG	1A	3452	1/1	0.95	0.10	48,48,48,48	0
58	MG	2A	3049	1/1	0.95	0.19	58,58,58,58	0
58	MG	2A	3711	1/1	0.95	0.20	41,41,41,41	0
58	MG	1A	3355	1/1	0.95	0.11	38,38,38,38	0
58	MG	2A	3713	1/1	0.95	0.15	33,33,33,33	0
58	MG	2a	1684	1/1	0.95	0.18	49,49,49,49	0
58	MG	1A	3782	1/1	0.95	0.12	32,32,32,32	0
58	MG	1A	3262	1/1	0.95	0.17	68,68,68,68	0
58	MG	1A	3421	1/1	0.95	0.13	47,47,47,47	0
58	MG	1A	3115	1/1	0.95	0.19	40,40,40,40	0
58	MG	1A	3058	1/1	0.95	0.21	22,22,22,22	0
58	MG	1A	4040	1/1	0.95	0.28	30,30,30,30	0
60	ZN	1Y	205	1/1	0.95	0.14	56,56,56,56	0
58	MG	2a	1693	1/1	0.95	0.13	58,58,58,58	0
58	MG	2a	1694	1/1	0.95	0.09	67,67,67,67	0
58	MG	1B	232	1/1	0.95	0.12	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3431	1/1	0.95	0.29	58,58,58,58	0
60	ZN	26	501	1/1	0.95	0.13	57,57,57,57	0
58	MG	1B	233	1/1	0.95	0.23	59,59,59,59	0
58	MG	2A	3724	1/1	0.95	0.20	52,52,52,52	0
61	SF4	1d	302	8/8	0.95	0.13	52,54,59,62	0
58	MG	1A	3198	1/1	0.95	0.22	26,26,26,26	0
58	MG	2A	3464	1/1	0.96	0.17	37,37,37,37	0
58	MG	1A	3202	1/1	0.96	0.28	20,20,20,20	0
58	MG	1A	3935	1/1	0.96	0.12	60,60,60,60	0
58	MG	1A	3203	1/1	0.96	0.17	29,29,29,29	0
58	MG	1A	3466	1/1	0.96	0.16	41,41,41,41	0
58	MG	1F	311	1/1	0.96	0.15	29,29,29,29	0
58	MG	2A	3173	1/1	0.96	0.11	39,39,39,39	0
58	MG	1A	3134	1/1	0.96	0.10	32,32,32,32	0
58	MG	1a	1732	1/1	0.96	0.09	40,40,40,40	0
58	MG	2A	3582	1/1	0.96	0.19	52,52,52,52	0
58	MG	2A	3583	1/1	0.96	0.24	46,46,46,46	0
58	MG	1a	1648	1/1	0.96	0.11	58,58,58,58	0
58	MG	2A	3273	1/1	0.96	0.31	73,73,73,73	0
58	MG	1t	201	1/1	0.96	0.17	49,49,49,49	0
58	MG	1A	3991	1/1	0.96	0.13	48,48,48,48	0
58	MG	2a	1623	1/1	0.96	0.14	55,55,55,55	0
58	MG	2A	3477	1/1	0.96	0.12	64,64,64,64	0
58	MG	1A	3090	1/1	0.96	0.35	43,43,43,43	0
58	MG	1a	1651	1/1	0.96	0.09	43,43,43,43	0
58	MG	1w	105	1/1	0.96	0.11	64,64,64,64	0
58	MG	1A	3831	1/1	0.96	0.14	39,39,39,39	0
58	MG	2A	3715	1/1	0.96	0.08	62,62,62,62	0
58	MG	1A	3136	1/1	0.96	0.15	21,21,21,21	0
58	MG	1A	4050	1/1	0.96	0.18	12,12,12,12	0
58	MG	1A	3037	1/1	0.96	0.20	19,19,19,19	0
58	MG	2A	3841	1/1	0.96	0.15	67,67,67,67	0
58	MG	1A	3236	1/1	0.96	0.18	27,27,27,27	0
58	MG	1A	3123	1/1	0.96	0.14	36,36,36,36	0
58	MG	1a	1744	1/1	0.96	0.07	58,58,58,58	0
58	MG	1A	3734	1/1	0.96	0.21	39,39,39,39	0
58	MG	2A	3094	1/1	0.96	0.10	40,40,40,40	0
58	MG	2A	3386	1/1	0.96	0.31	43,43,43,43	0
58	MG	2A	3849	1/1	0.96	0.25	57,57,57,57	0
58	MG	1A	3162	1/1	0.96	0.16	48,48,48,48	0
58	MG	1A	3611	1/1	0.96	0.18	24,24,24,24	0
58	MG	1A	3265	1/1	0.96	0.27	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	15	103	1/1	0.96	0.16	33,33,33,33	0
58	MG	1a	1750	1/1	0.96	0.17	52,52,52,52	0
58	MG	2A	3498	1/1	0.96	0.18	65,65,65,65	0
58	MG	1O	202	1/1	0.96	0.12	42,42,42,42	0
58	MG	1A	3575	1/1	0.96	0.47	34,34,34,34	0
58	MG	1A	3652	1/1	0.96	0.18	22,22,22,22	0
58	MG	1B	219	1/1	0.96	0.19	41,41,41,41	0
58	MG	17	101	1/1	0.96	0.19	25,25,25,25	0
58	MG	17	103	1/1	0.96	0.19	35,35,35,35	0
58	MG	2A	3738	1/1	0.96	0.24	65,65,65,65	0
58	MG	1A	3028	1/1	0.96	0.15	27,27,27,27	0
58	MG	1A	3654	1/1	0.96	0.19	27,27,27,27	0
58	MG	1A	4063	1/1	0.96	0.15	38,38,38,38	0
58	MG	1A	4064	1/1	0.96	0.22	28,28,28,28	0
58	MG	1Q	201	1/1	0.96	0.32	38,38,38,38	0
58	MG	1A	3297	1/1	0.96	0.17	56,56,56,56	0
58	MG	2A	3012	1/1	0.96	0.12	39,39,39,39	0
58	MG	2A	3624	1/1	0.96	0.12	58,58,58,58	0
58	MG	1A	3084	1/1	0.96	0.25	39,39,39,39	0
58	MG	1A	3580	1/1	0.96	0.21	28,28,28,28	0
58	MG	2D	301	1/1	0.96	0.15	34,34,34,34	0
58	MG	1A	3794	1/1	0.96	0.15	25,25,25,25	0
58	MG	1A	4070	1/1	0.96	0.16	37,37,37,37	0
58	MG	2A	3411	1/1	0.96	0.16	59,59,59,59	0
58	MG	2A	3752	1/1	0.96	0.12	36,36,36,36	0
58	MG	1A	3700	1/1	0.96	0.15	47,47,47,47	0
58	MG	1A	3144	1/1	0.96	0.20	37,37,37,37	0
58	MG	2a	1671	1/1	0.96	0.15	41,41,41,41	0
58	MG	1A	3389	1/1	0.96	0.23	31,31,31,31	0
58	MG	1A	3214	1/1	0.96	0.17	34,34,34,34	0
58	MG	1A	3751	1/1	0.96	0.22	50,50,50,50	0
58	MG	2A	3024	1/1	0.96	0.20	44,44,44,44	0
58	MG	1a	1685	1/1	0.96	0.17	33,33,33,33	0
58	MG	1A	3215	1/1	0.96	0.18	38,38,38,38	0
58	MG	2A	3319	1/1	0.96	0.35	51,51,51,51	0
58	MG	1T	201	1/1	0.96	0.12	55,55,55,55	0
58	MG	1T	202	1/1	0.96	0.12	49,49,49,49	0
58	MG	2A	3764	1/1	0.96	0.12	50,50,50,50	0
58	MG	1A	3802	1/1	0.96	0.23	24,24,24,24	0
58	MG	1A	3753	1/1	0.96	0.22	41,41,41,41	0
58	MG	2A	3130	1/1	0.96	0.21	35,35,35,35	0
58	MG	1A	3166	1/1	0.96	0.21	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	3913	1/1	0.96	0.18	45,45,45,45	0
58	MG	1a	1614	1/1	0.96	0.08	45,45,45,45	0
58	MG	1A	3860	1/1	0.96	0.21	21,21,21,21	0
58	MG	2A	3231	1/1	0.96	0.20	54,54,54,54	0
58	MG	2A	3538	1/1	0.96	0.16	47,47,47,47	0
58	MG	2A	3539	1/1	0.96	0.12	38,38,38,38	0
58	MG	2A	3776	1/1	0.96	0.27	66,66,66,66	0
58	MG	1A	3624	1/1	0.96	0.22	26,26,26,26	0
58	MG	2f	202	1/1	0.96	0.29	66,66,66,66	0
58	MG	1A	3806	1/1	0.96	0.14	45,45,45,45	0
58	MG	1D	306	1/1	0.96	0.23	18,18,18,18	0
58	MG	1U	209	1/1	0.96	0.12	32,32,32,32	0
58	MG	2A	3658	1/1	0.96	0.09	32,32,32,32	0
58	MG	1V	202	1/1	0.96	0.20	37,37,37,37	0
58	MG	1A	3145	1/1	0.96	0.17	27,27,27,27	0
58	MG	1D	309	1/1	0.96	0.12	33,33,33,33	0
58	MG	1A	3666	1/1	0.96	0.15	22,22,22,22	0
58	MG	2A	3664	1/1	0.96	0.09	49,49,49,49	0
58	MG	1a	1793	1/1	0.96	0.18	58,58,58,58	0
58	MG	2A	3549	1/1	0.96	0.25	39,39,39,39	0
58	MG	1D	311	1/1	0.96	0.21	38,38,38,38	0
58	MG	2A	3668	1/1	0.96	0.12	63,63,63,63	0
58	MG	1A	3758	1/1	0.96	0.15	25,25,25,25	0
58	MG	2A	3148	1/1	0.96	0.25	36,36,36,36	0
58	MG	2A	3553	1/1	0.96	0.15	40,40,40,40	0
58	MG	1A	3071	1/1	0.96	0.20	15,15,15,15	0
58	MG	2l	101	1/1	0.96	0.38	55,55,55,55	0
58	MG	1A	3589	1/1	0.96	0.17	29,29,29,29	0
58	MG	2A	3796	1/1	0.96	0.17	36,36,36,36	0
58	MG	1A	3008	1/1	0.96	0.19	20,20,20,20	0
58	MG	1A	3221	1/1	0.96	0.21	33,33,33,33	0
58	MG	1A	3025	1/1	0.96	0.12	25,25,25,25	0
58	MG	1A	3042	1/1	0.96	0.18	27,27,27,27	0
58	MG	1A	3278	1/1	0.96	0.18	28,28,28,28	0
58	MG	1A	3119	1/1	0.96	0.23	33,33,33,33	0
58	MG	28	101	1/1	0.96	0.17	58,58,58,58	0
58	MG	1a	1804	1/1	0.96	0.11	52,52,52,52	0
58	MG	1A	4036	1/1	0.96	0.21	29,29,29,29	0
58	MG	1A	3132	1/1	0.96	0.13	33,33,33,33	0
58	MG	1A	3820	1/1	0.96	0.25	24,24,24,24	0
58	MG	2A	3687	1/1	0.96	0.09	68,68,68,68	0
58	MG	1A	3200	1/1	0.96	0.23	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	10	103	1/1	0.96	0.21	32,32,32,32	0
58	MG	10	104	1/1	0.96	0.24	41,41,41,41	0
58	MG	2a	1733	1/1	0.96	0.22	55,55,55,55	0
58	MG	2A	3069	1/1	0.96	0.12	42,42,42,42	0
58	MG	1F	305	1/1	0.96	0.21	30,30,30,30	0
58	MG	1A	3110	1/1	0.96	0.24	27,27,27,27	0
58	MG	1A	3604	1/1	0.97	0.24	41,41,41,41	0
58	MG	1a	1781	1/1	0.97	0.06	44,44,44,44	0
58	MG	1A	3921	1/1	0.97	0.20	36,36,36,36	0
58	MG	1A	3140	1/1	0.97	0.10	26,26,26,26	0
58	MG	2A	3662	1/1	0.97	0.27	56,56,56,56	0
58	MG	1A	3387	1/1	0.97	0.20	30,30,30,30	0
58	MG	2A	3766	1/1	0.97	0.16	52,52,52,52	0
58	MG	1P	201	1/1	0.97	0.15	29,29,29,29	0
58	MG	2D	303	1/1	0.97	0.19	43,43,43,43	0
58	MG	1A	3534	1/1	0.97	0.24	51,51,51,51	0
58	MG	1A	3778	1/1	0.97	0.15	28,28,28,28	0
58	MG	1P	205	1/1	0.97	0.25	30,30,30,30	0
58	MG	2A	3023	1/1	0.97	0.18	38,38,38,38	0
58	MG	1A	3127	1/1	0.97	0.18	35,35,35,35	0
58	MG	2E	303	1/1	0.97	0.13	48,48,48,48	0
58	MG	2A	3109	1/1	0.97	0.11	49,49,49,49	0
58	MG	2A	3025	1/1	0.97	0.11	38,38,38,38	0
58	MG	1A	3474	1/1	0.97	0.16	42,42,42,42	0
58	MG	2A	3673	1/1	0.97	0.20	46,46,46,46	0
58	MG	2A	3674	1/1	0.97	0.27	57,57,57,57	0
58	MG	1A	3064	1/1	0.97	0.26	39,39,39,39	0
58	MG	1Q	202	1/1	0.97	0.21	36,36,36,36	0
58	MG	1A	3390	1/1	0.97	0.14	49,49,49,49	0
58	MG	2A	3030	1/1	0.97	0.17	44,44,44,44	0
58	MG	1A	3882	1/1	0.97	0.17	28,28,28,28	0
58	MG	2A	3032	1/1	0.97	0.12	39,39,39,39	0
58	MG	15	105	1/1	0.97	0.11	30,30,30,30	0
58	MG	2a	1781	1/1	0.97	0.20	72,72,72,72	0
58	MG	2A	3682	1/1	0.97	0.23	67,67,67,67	0
58	MG	1A	3931	1/1	0.97	0.21	50,50,50,50	0
58	MG	2A	3035	1/1	0.97	0.11	42,42,42,42	0
58	MG	2A	3036	1/1	0.97	0.21	22,22,22,22	0
58	MG	2A	3486	1/1	0.97	0.10	44,44,44,44	0
58	MG	1A	3650	1/1	0.97	0.23	25,25,25,25	0
58	MG	1A	3834	1/1	0.97	0.18	47,47,47,47	0
58	MG	1a	1726	1/1	0.97	0.12	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3612	1/1	0.97	0.18	42,42,42,42	0
58	MG	1A	3286	1/1	0.97	0.13	33,33,33,33	0
58	MG	1A	3509	1/1	0.97	0.10	42,42,42,42	0
58	MG	2A	3398	1/1	0.97	0.18	54,54,54,54	0
58	MG	2A	3043	1/1	0.97	0.22	63,63,63,63	0
58	MG	1A	3363	1/1	0.97	0.16	31,31,31,31	0
58	MG	1a	1731	1/1	0.97	0.15	37,37,37,37	0
58	MG	2A	3046	1/1	0.97	0.09	38,38,38,38	0
58	MG	1D	308	1/1	0.97	0.20	28,28,28,28	0
58	MG	1a	1733	1/1	0.97	0.21	57,57,57,57	0
58	MG	1A	3160	1/1	0.97	0.13	19,19,19,19	0
58	MG	2a	1687	1/1	0.97	0.14	59,59,59,59	0
58	MG	2A	3701	1/1	0.97	0.16	35,35,35,35	0
58	MG	1A	3579	1/1	0.97	0.24	34,34,34,34	0
58	MG	2A	3806	1/1	0.97	0.12	35,35,35,35	0
58	MG	1A	3036	1/1	0.97	0.19	41,41,41,41	0
58	MG	1A	3106	1/1	0.97	0.15	33,33,33,33	0
58	MG	2A	3809	1/1	0.97	0.13	51,51,51,51	0
58	MG	1A	3023	1/1	0.97	0.17	13,13,13,13	0
58	MG	2A	3316	1/1	0.97	0.16	44,44,44,44	0
58	MG	2A	3227	1/1	0.97	0.17	39,39,39,39	0
58	MG	2A	3139	1/1	0.97	0.17	40,40,40,40	0
58	MG	2a	1812	1/1	0.97	0.11	57,57,57,57	0
58	MG	1A	3247	1/1	0.97	0.16	33,33,33,33	0
58	MG	1A	3226	1/1	0.97	0.17	23,23,23,23	0
58	MG	1e	202	1/1	0.97	0.21	49,49,49,49	0
58	MG	1A	3750	1/1	0.97	0.20	16,16,16,16	0
58	MG	2A	3513	1/1	0.97	0.16	23,23,23,23	0
58	MG	1A	4101	1/1	0.97	0.06	50,50,50,50	0
58	MG	1E	306	1/1	0.97	0.20	29,29,29,29	0
58	MG	1A	3797	1/1	0.97	0.18	46,46,46,46	0
58	MG	1A	3293	1/1	0.97	0.17	32,32,32,32	0
58	MG	1U	210	1/1	0.97	0.24	32,32,32,32	0
58	MG	1V	201	1/1	0.97	0.23	27,27,27,27	0
58	MG	1A	3586	1/1	0.97	0.16	44,44,44,44	0
58	MG	2A	3065	1/1	0.97	0.19	52,52,52,52	0
58	MG	1A	3044	1/1	0.97	0.12	31,31,31,31	0
58	MG	1a	1677	1/1	0.97	0.11	58,58,58,58	0
58	MG	2A	3620	1/1	0.97	0.19	51,51,51,51	0
58	MG	1A	4000	1/1	0.97	0.12	33,33,33,33	0
58	MG	1w	104	1/1	0.97	0.12	64,64,64,64	0
58	MG	1A	3038	1/1	0.97	0.13	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2a	1718	1/1	0.97	0.06	64,64,64,64	0
58	MG	2A	3246	1/1	0.97	0.18	53,53,53,53	0
58	MG	1F	301	1/1	0.97	0.16	35,35,35,35	0
58	MG	1F	302	1/1	0.97	0.19	30,30,30,30	0
58	MG	2A	3731	1/1	0.97	0.17	48,48,48,48	0
58	MG	1A	3551	1/1	0.97	0.18	32,32,32,32	0
58	MG	1A	3098	1/1	0.97	0.21	18,18,18,18	0
58	MG	2A	3075	1/1	0.97	0.19	22,22,22,22	0
58	MG	2A	3533	1/1	0.97	0.15	43,43,43,43	0
58	MG	1A	3553	1/1	0.97	0.16	27,27,27,27	0
58	MG	2A	3843	1/1	0.97	0.19	47,47,47,47	0
58	MG	1A	3151	1/1	0.97	0.13	32,32,32,32	0
58	MG	2A	3254	1/1	0.97	0.12	47,47,47,47	0
58	MG	1A	4057	1/1	0.97	0.18	18,18,18,18	0
58	MG	1A	3021	1/1	0.97	0.17	20,20,20,20	0
58	MG	1A	3172	1/1	0.97	0.14	27,27,27,27	0
58	MG	1A	3673	1/1	0.97	0.14	26,26,26,26	0
58	MG	1A	3191	1/1	0.97	0.18	30,30,30,30	0
58	MG	1A	3861	1/1	0.97	0.18	24,24,24,24	0
58	MG	1a	1766	1/1	0.97	0.15	44,44,44,44	0
58	MG	2A	3643	1/1	0.97	0.17	38,38,38,38	0
58	MG	1A	3047	1/1	0.97	0.17	20,20,20,20	0
58	MG	10	101	1/1	0.97	0.13	37,37,37,37	0
59	K	1A	3562	1/1	0.97	0.19	43,43,43,43	0
58	MG	1A	3302	1/1	0.97	0.29	34,34,34,34	0
58	MG	1A	3137	1/1	0.97	0.27	33,33,33,33	0
58	MG	1A	4014	1/1	0.97	0.12	59,59,59,59	0
60	ZN	15	108	1/1	0.97	0.06	41,41,41,41	0
60	ZN	16	102	1/1	0.97	0.16	40,40,40,40	0
58	MG	1B	220	1/1	0.97	0.18	49,49,49,49	0
58	MG	1A	3722	1/1	0.97	0.14	34,34,34,34	0
58	MG	1A	3279	1/1	0.97	0.16	34,34,34,34	0
60	ZN	25	104	1/1	0.97	0.07	59,59,59,59	0
58	MG	1N	202	1/1	0.97	0.16	46,46,46,46	0
58	MG	1A	3680	1/1	0.97	0.25	27,27,27,27	0
58	MG	1A	3072	1/1	0.97	0.49	31,31,31,31	0
58	MG	1A	3031	1/1	0.97	0.20	25,25,25,25	0
58	MG	1A	3218	1/1	0.97	0.22	40,40,40,40	0
58	MG	1a	1716	1/1	0.98	0.21	29,29,29,29	0
58	MG	2D	305	1/1	0.98	0.23	29,29,29,29	0
58	MG	2A	3396	1/1	0.98	0.28	48,48,48,48	0
58	MG	1A	3873	1/1	0.98	0.21	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3630	1/1	0.98	0.16	39,39,39,39	0
58	MG	1A	3085	1/1	0.98	0.11	28,28,28,28	0
58	MG	1A	3108	1/1	0.98	0.19	37,37,37,37	0
58	MG	2A	3457	1/1	0.98	0.14	19,19,19,19	0
58	MG	1A	3003	1/1	0.98	0.24	23,23,23,23	0
58	MG	1A	3844	1/1	0.98	0.11	46,46,46,46	0
58	MG	1A	3812	1/1	0.98	0.17	18,18,18,18	0
58	MG	2A	3823	1/1	0.98	0.17	23,23,23,23	0
58	MG	1A	3232	1/1	0.98	0.14	44,44,44,44	0
58	MG	1A	3661	1/1	0.98	0.17	43,43,43,43	0
58	MG	1a	1725	1/1	0.98	0.23	56,56,56,56	0
58	MG	1A	3735	1/1	0.98	0.12	48,48,48,48	0
58	MG	1E	303	1/1	0.98	0.11	28,28,28,28	0
58	MG	2A	3140	1/1	0.98	0.16	32,32,32,32	0
58	MG	2F	305	1/1	0.98	0.26	47,47,47,47	0
58	MG	1A	3477	1/1	0.98	0.18	42,42,42,42	0
58	MG	1W	203	1/1	0.98	0.19	31,31,31,31	0
58	MG	17	102	1/1	0.98	0.22	29,29,29,29	0
58	MG	1W	204	1/1	0.98	0.21	34,34,34,34	0
58	MG	1P	202	1/1	0.98	0.18	27,27,27,27	0
58	MG	1A	3146	1/1	0.98	0.18	32,32,32,32	0
58	MG	2A	3649	1/1	0.98	0.14	41,41,41,41	0
58	MG	2A	3360	1/1	0.98	0.39	55,55,55,55	0
58	MG	1X	103	1/1	0.98	0.18	35,35,35,35	0
58	MG	1A	3061	1/1	0.98	0.15	36,36,36,36	0
58	MG	1A	3712	1/1	0.98	0.19	38,38,38,38	0
58	MG	1A	3792	1/1	0.98	0.07	35,35,35,35	0
58	MG	1A	3043	1/1	0.98	0.26	35,35,35,35	0
58	MG	1Y	204	1/1	0.98	0.40	39,39,39,39	0
58	MG	1A	3987	1/1	0.98	0.20	29,29,29,29	0
58	MG	1A	3192	1/1	0.98	0.16	27,27,27,27	0
58	MG	1Q	203	1/1	0.98	0.20	24,24,24,24	0
58	MG	1A	3767	1/1	0.98	0.12	37,37,37,37	0
58	MG	1A	3825	1/1	0.98	0.15	20,20,20,20	0
58	MG	2A	3158	1/1	0.98	0.12	37,37,37,37	0
58	MG	1A	3099	1/1	0.98	0.13	36,36,36,36	0
58	MG	2A	3487	1/1	0.98	0.24	27,27,27,27	0
58	MG	1F	303	1/1	0.98	0.23	28,28,28,28	0
58	MG	1A	3141	1/1	0.98	0.25	13,13,13,13	0
58	MG	1A	3195	1/1	0.98	0.17	38,38,38,38	0
58	MG	1A	3196	1/1	0.98	0.21	30,30,30,30	0
58	MG	2A	3607	1/1	0.98	0.09	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3346	1/1	0.98	0.11	35,35,35,35	0
58	MG	1a	1610	1/1	0.98	0.20	23,23,23,23	0
58	MG	1A	3033	1/1	0.98	0.23	30,30,30,30	0
58	MG	1A	3833	1/1	0.98	0.16	39,39,39,39	0
58	MG	1A	3566	1/1	0.98	0.16	28,28,28,28	0
58	MG	1A	3397	1/1	0.98	0.16	26,26,26,26	0
58	MG	1A	3380	1/1	0.98	0.14	25,25,25,25	0
58	MG	1A	3173	1/1	0.98	0.19	29,29,29,29	0
58	MG	1D	301	1/1	0.98	0.16	32,32,32,32	0
58	MG	1A	3591	1/1	0.98	0.19	31,31,31,31	0
58	MG	2a	1727	1/1	0.98	0.42	47,47,47,47	0
58	MG	2A	3559	1/1	0.98	0.14	46,46,46,46	0
58	MG	2A	3019	1/1	0.98	0.13	23,23,23,23	0
58	MG	1a	1760	1/1	0.98	0.11	48,48,48,48	0
58	MG	2A	3621	1/1	0.98	0.13	39,39,39,39	0
58	MG	1A	3870	1/1	0.98	0.10	19,19,19,19	0
58	MG	1A	3678	1/1	0.98	0.18	27,27,27,27	0
58	MG	1A	4074	1/1	0.98	0.19	53,53,53,53	0
58	MG	1a	1714	1/1	0.98	0.19	41,41,41,41	0
58	MG	1A	3161	1/1	0.98	0.24	24,24,24,24	0
58	MG	2a	1770	1/1	0.99	0.12	51,51,51,51	0
58	MG	1A	3647	1/1	0.99	0.22	17,17,17,17	0
58	MG	1A	3729	1/1	0.99	0.24	42,42,42,42	0
58	MG	1A	3826	1/1	0.99	0.14	34,34,34,34	0
58	MG	1V	203	1/1	0.99	0.16	25,25,25,25	0
58	MG	1A	3720	1/1	0.99	0.18	13,13,13,13	0
58	MG	1A	3498	1/1	0.99	0.08	50,50,50,50	0
58	MG	1A	3210	1/1	0.99	0.21	28,28,28,28	0
58	MG	2A	3441	1/1	0.99	0.33	51,51,51,51	0
58	MG	1A	3171	1/1	0.99	0.13	19,19,19,19	0
58	MG	1A	3169	1/1	0.99	0.23	11,11,11,11	0
60	ZN	19	102	1/1	0.99	0.16	38,38,38,38	0
58	MG	1Q	205	1/1	0.99	0.25	56,56,56,56	0
58	MG	2A	3359	1/1	0.99	0.16	30,30,30,30	0
58	MG	1A	3708	1/1	0.99	0.12	15,15,15,15	0
58	MG	1A	4067	1/1	0.99	0.16	19,19,19,19	0
58	MG	1A	3065	1/1	0.99	0.27	39,39,39,39	0
58	MG	2a	1690	1/1	0.99	0.27	36,36,36,36	0
58	MG	1A	3777	1/1	0.99	0.20	24,24,24,24	0
58	MG	1A	3822	1/1	0.99	0.16	24,24,24,24	0
58	MG	1A	3574	1/1	0.99	0.14	31,31,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.