



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 7, 2022 – 07:39 PM EDT

PDB ID : 7U2J
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with mRNA, aminoacylated A-site Gly-NH-tRNA^{Gly}, peptidyl P-site fMAC-NH-tRNA^{Met}, deacylated E-site tRNA^{Gly}, and chloramphenicol at 2.55Å resolution
Authors : Syroegin, E.A.; Aleksandrova, E.V.; Polikanov, Y.S.
Deposited on : 2022-02-24
Resolution : 2.55 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	:	2.29
buster-report	:	1.1.7 (2018)
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)	:	2.29

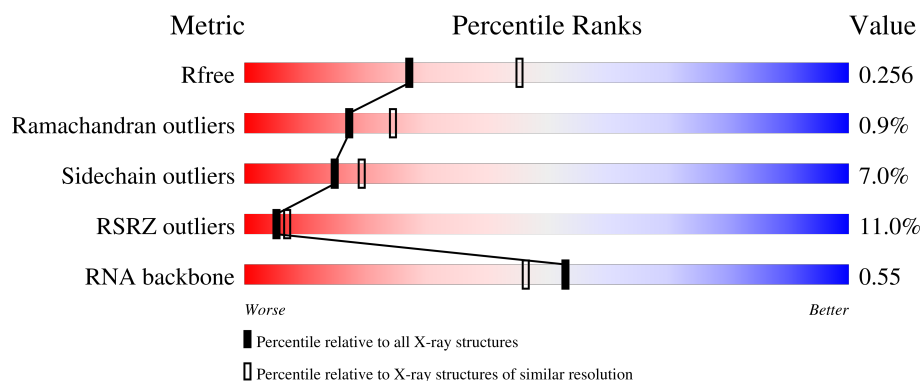
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1284 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)
RNA backbone	3102	1026 (2.88-2.20)

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

Mol	Chain	Length	Quality of chain
1	1A	2915	<div> <div>5%</div> <div>82%</div> <div>16%</div> <div>..</div> </div>
1	2A	2915	<div> <div>4%</div> <div>80%</div> <div>16%</div> <div>..</div> </div>
2	1B	121	<div> <div>90%</div> <div>9%</div> <div>.</div> </div>
2	2B	121	<div> <div>77%</div> <div>22%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
3	1D	276	<div> <div></div> <div>96%</div> <div></div> </div>
3	2D	276	<div> <div></div> <div>97%</div> <div></div> </div>
4	1E	206	<div> <div></div> <div>94%</div> <div>5%</div> </div>
4	2E	206	<div> <div></div> <div>96%</div> <div></div> </div>
5	1F	210	<div> <div></div> <div>90%</div> <div>6%</div> </div>
5	2F	210	<div> <div></div> <div>91%</div> <div>5%</div> </div>
6	1G	182	<div> <div></div> <div>93%</div> <div>6%</div> </div>
6	2G	182	<div> <div></div> <div>86%</div> <div>14%</div> </div>
7	1H	180	<div> <div></div> <div>92%</div> <div>5%</div> </div>
7	2H	180	<div> <div></div> <div>88%</div> <div>8%</div> </div>
8	1I	148	<div> <div></div> <div>91%</div> <div>7%</div> </div>
8	2I	148	<div> <div></div> <div>86%</div> <div>12%</div> </div>
9	1N	140	<div> <div></div> <div>96%</div> <div></div> </div>
9	2N	140	<div> <div></div> <div>93%</div> <div>7%</div> </div>
10	1O	122	<div> <div></div> <div>98%</div> <div></div> </div>
10	2O	122	<div> <div></div> <div>98%</div> <div></div> </div>
11	1P	150	<div> <div></div> <div>95%</div> <div>5%</div> </div>
11	2P	150	<div> <div></div> <div>96%</div> <div></div> </div>
12	1Q	141	<div> <div></div> <div>96%</div> <div></div> </div>
12	2Q	141	<div> <div></div> <div>94%</div> <div>6%</div> </div>
13	1R	118	<div> <div></div> <div>97%</div> <div></div> </div>
13	2R	118	<div> <div></div> <div>99%</div> <div></div> </div>
14	1S	112	<div> <div></div> <div>95%</div> <div></div> </div>
14	2S	112	<div> <div></div> <div>90%</div> <div>8%</div> </div>
15	1T	146	<div> <div></div> <div>86%</div> <div>10%</div> </div>



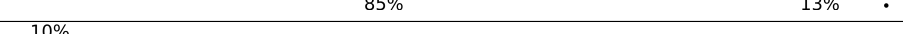


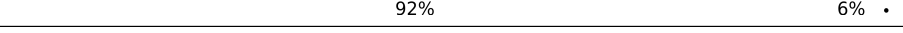

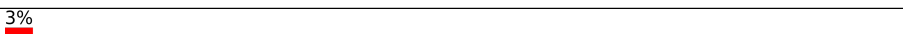

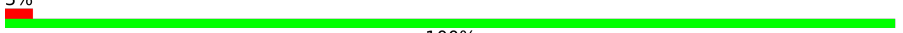
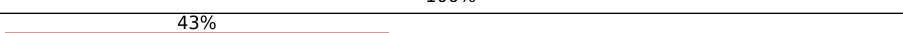
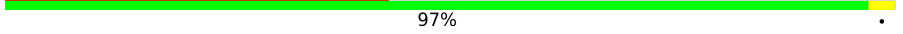

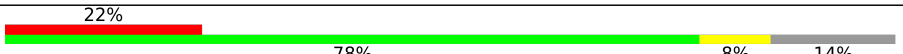
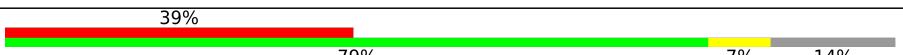
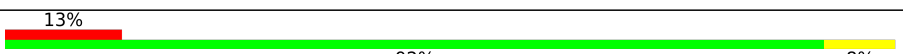
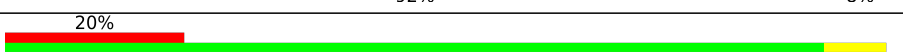
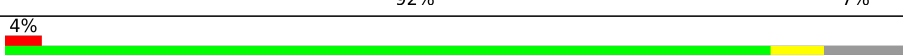







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Mol	Chain	Length	Quality of chain
15	2T	146	<div> <div>5%</div> <div>86%</div> <div>10%</div> </div>
16	1U	118	<div> <div>2%</div> <div>96%</div> <div></div> </div>
16	2U	118	<div> <div>4%</div> <div>94%</div> <div></div> </div>
17	1V	101	<div> <div>%</div> <div>98%</div> <div></div> </div>
17	2V	101	<div> <div>10%</div> <div>93%</div> <div>7%</div> </div>
18	1W	113	<div> <div>%</div> <div>94%</div> <div>5%</div> </div>
18	2W	113	<div> <div>3%</div> <div>96%</div> <div></div> </div>
19	1X	96	<div> <div>2%</div> <div>98%</div> <div></div> </div>
19	2X	96	<div> <div>4%</div> <div>98%</div> <div></div> </div>
20	1Y	110	<div> <div>2%</div> <div>88%</div> <div>9%</div> </div>
20	2Y	110	<div> <div>11%</div> <div>91%</div> <div>6%</div> </div>
21	1Z	206	<div> <div>9%</div> <div>68%</div> <div>6%</div> <div>25%</div> </div>
21	2Z	206	<div> <div>36%</div> <div>71%</div> <div>7%</div> <div>22%</div> </div>
22	10	85	<div> <div>%</div> <div>96%</div> <div></div> </div>
22	20	85	<div> <div>5%</div> <div>94%</div> <div></div> </div>
23	11	98	<div> <div>6%</div> <div>95%</div> <div></div> </div>
23	21	98	<div> <div>2%</div> <div>96%</div> <div></div> </div>
24	12	72	<div> <div></div> <div>92%</div> <div>6%</div> </div>
24	22	72	<div> <div>8%</div> <div>93%</div> <div></div> </div>
25	13	60	<div> <div></div> <div>95%</div> <div></div> </div>
25	23	60	<div> <div>20%</div> <div>93%</div> <div>5%</div> </div>
26	14	71	<div> <div>21%</div> <div>86%</div> <div>8%</div> </div>
26	24	71	<div> <div>51%</div> <div>82%</div> <div>15%</div> </div>
27	15	60	<div> <div>2%</div> <div>92%</div> <div>7%</div> </div>
27	25	60	<div> <div>3%</div> <div>93%</div> <div>5%</div> </div>

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Mol	Chain	Length	Quality of chain
28	16	54	 93% 6% .
28	26	54	 85% 13% . 2%
29	17	49	 90% 8% . 10%
29	27	49	 92% 6% . 10%
30	18	65	 91% 8% .
30	28	65	 91% 8% . 3%
31	19	37	 100% 3%
31	29	37	 97% . 43%
32	1a	1521	 81% 18% . 4%
32	2a	1521	 79% 19% . 5%
33	1b	256	 82% 9% 10% 14%
33	2b	256	 79% 11% 10% 36%
34	1c	239	 78% 8% 14% 22%
34	2c	239	 79% 7% 14% 39%
35	1d	209	 92% 8% 13%
35	2d	209	 92% 7% 20%
36	1e	162	 86% 6% 9% 4%
36	2e	162	 80% 12% 9% 24%
37	1f	101	 94% 5% . 8%
37	2f	101	 93% 6% . 4%
38	1g	156	 92% 7% . 19%
38	2g	156	 92% 7% .. 36%
39	1h	138	 94% 5% . 4%
39	2h	138	 92% 7% . 13%
40	1i	128	 89% 9% .. 41%

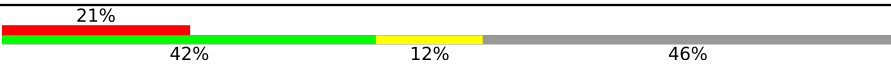
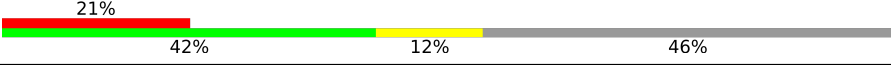
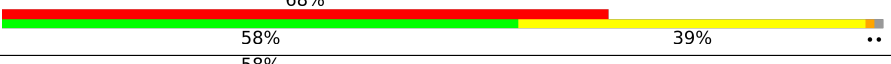


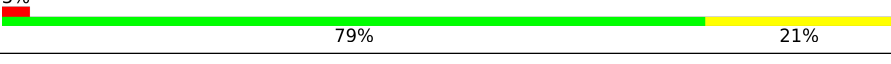
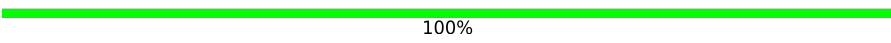


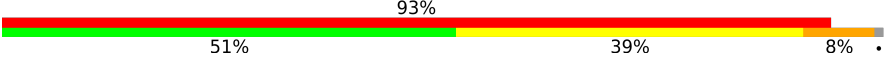
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Mol	Chain	Length	Quality of chain
40	2i	128	
41	1j	105	
41	2j	105	
42	1k	129	
42	2k	129	
43	1l	132	
43	2l	132	
44	1m	126	
44	2m	126	
45	1n	61	
45	2n	61	
46	1o	89	
46	2o	89	
47	1p	88	
47	2p	88	
48	1q	105	
48	2q	105	
49	1r	88	
49	2r	88	
50	1s	93	
50	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	74	
54	2w	74	
55	1x	77	
55	2x	77	
56	1z	3	
56	2z	3	
57	1y	74	
57	2y	74	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	5MU	1y	54	-	-	-	X
57	PSU	1y	55	-	-	-	X
57	5MU	2y	54	-	-	-	X
57	PSU	2y	55	-	-	-	X
58	MG	1A	3148	-	-	-	X
58	MG	1A	3245	-	-	-	X
58	MG	1A	3254	-	-	-	X
58	MG	1A	3352	-	-	-	X
58	MG	1A	3365	-	-	-	X
58	MG	1A	3369	-	-	-	X
58	MG	1A	3371	-	-	-	X
58	MG	1A	3395	-	-	-	X
58	MG	1A	3396	-	-	-	X
58	MG	1A	3412	-	-	-	X
58	MG	1A	3436	-	-	-	X
58	MG	1A	3448	-	-	-	X
58	MG	1A	3480	-	-	-	X
58	MG	1A	3489	-	-	-	X
58	MG	1A	3512	-	-	-	X
58	MG	1A	3521	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	MG	1A	3524	-	-	-	X
58	MG	1A	4051	-	-	-	X
58	MG	1x	101	-	-	-	X
58	MG	1x	103	-	-	-	X
58	MG	20	101	-	-	-	X
58	MG	2A	3051	-	-	-	X
58	MG	2A	3080	-	-	-	X
58	MG	2A	3137	-	-	-	X
58	MG	2A	3190	-	-	-	X
58	MG	2A	3194	-	-	-	X
58	MG	2A	3204	-	-	-	X
58	MG	2A	3207	-	-	-	X
58	MG	2A	3219	-	-	-	X
58	MG	2A	3284	-	-	-	X
58	MG	2A	3319	-	-	-	X
58	MG	2A	3365	-	-	-	X
58	MG	2A	3395	-	-	-	X
58	MG	2A	3413	-	-	-	X
58	MG	2A	3693	-	-	-	X
58	MG	2a	1631	-	-	-	X
58	MG	2a	1666	-	-	-	X
58	MG	2a	1778	-	-	-	X

2 Entry composition

There are 63 unique types of molecules in this entry. The entry contains 299751 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 MG-mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1v	13	Total	C	N	O	P	0	0	0
			286	128	59	86	13			
53	2v	13	Total	C	N	O	P	0	0	0
			286	128	59	86	13			

- Molecule 54 is a RNA chain called A-site Aminoacyl-tRNA Gly-NH-tRNAgly.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
54	1w	73	Total	C	N	O	P	S	0	0	0
			1556	695	275	512	73	1			
54	2w	72	Total	C	N	O	P	S	0	0	0
			1536	686	273	504	72	1			

- Molecule 55 is a RNA chain called P-site Peptidyl-tRNA fMAC-NH-tRNAmet 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 fMAC-NH-tRNAmet Peptide-part.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	1z	3	Total	C	N	O	S	0	0	0
			21	12	3	4	2			
56	2z	3	Total	C	N	O	S	0	0	0
			21	12	3	4	2			

- Molecule 57 is a RNA chain called E-site Deacylated tRNAgly.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
57	1y	73	Total	C	N	O	P	S	0	0	0
			1552	693	273	512	73	1			
57	2y	73	Total	C	N	O	P	S	0	0	0
			1552	693	273	512	73	1			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1A	1085	Total	Mg	0	0
			1085	1085		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1B	37	Total 37	Mg 37	0	0
58	1D	11	Total 11	Mg 11	0	0
58	1E	15	Total 15	Mg 15	0	0
58	1F	11	Total 11	Mg 11	0	0
58	1G	4	Total 4	Mg 4	0	0
58	1H	1	Total 1	Mg 1	0	0
58	1I	1	Total 1	Mg 1	0	0
58	1N	5	Total 5	Mg 5	0	0
58	1O	6	Total 6	Mg 6	0	0
58	1P	5	Total 5	Mg 5	0	0
58	1Q	8	Total 8	Mg 8	0	0
58	1R	7	Total 7	Mg 7	0	0
58	1S	3	Total 3	Mg 3	0	0
58	1T	2	Total 2	Mg 2	0	0
58	1U	10	Total 10	Mg 10	0	0
58	1V	6	Total 6	Mg 6	0	0
58	1W	7	Total 7	Mg 7	0	0
58	1X	6	Total 6	Mg 6	0	0
58	1Y	3	Total 3	Mg 3	0	0
58	1Z	3	Total 3	Mg 3	0	0
58	10	8	Total 8	Mg 8	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	11	4	Total 4	Mg 4	0	0
58	12	2	Total 2	Mg 2	0	0
58	13	4	Total 4	Mg 4	0	0
58	15	8	Total 8	Mg 8	0	0
58	16	3	Total 3	Mg 3	0	0
58	17	5	Total 5	Mg 5	0	0
58	18	6	Total 6	Mg 6	0	0
58	19	1	Total 1	Mg 1	0	0
58	1a	214	Total 214	Mg 214	0	0
58	1b	2	Total 2	Mg 2	0	0
58	1d	1	Total 1	Mg 1	0	0
58	1e	3	Total 3	Mg 3	0	0
58	1f	2	Total 2	Mg 2	0	0
58	1k	1	Total 1	Mg 1	0	0
58	1l	2	Total 2	Mg 2	0	0
58	1m	1	Total 1	Mg 1	0	0
58	1n	2	Total 2	Mg 2	0	0
58	1p	1	Total 1	Mg 1	0	0
58	1s	1	Total 1	Mg 1	0	0
58	1t	1	Total 1	Mg 1	0	0
58	1w	9	Total 9	Mg 9	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1x	12	Total 12	Mg 12	0	0
58	1y	1	Total 1	Mg 1	0	0
58	2A	800	Total 800	Mg 800	0	0
58	2B	18	Total 18	Mg 18	0	0
58	2D	5	Total 5	Mg 5	0	0
58	2E	8	Total 8	Mg 8	0	0
58	2F	8	Total 8	Mg 8	0	0
58	2G	1	Total 1	Mg 1	0	0
58	2N	1	Total 1	Mg 1	0	0
58	2O	1	Total 1	Mg 1	0	0
58	2Q	3	Total 3	Mg 3	0	0
58	2R	2	Total 2	Mg 2	0	0
58	2T	4	Total 4	Mg 4	0	0
58	2U	1	Total 1	Mg 1	0	0
58	2V	1	Total 1	Mg 1	0	0
58	2W	2	Total 2	Mg 2	0	0
58	2X	1	Total 1	Mg 1	0	0
58	2Y	1	Total 1	Mg 1	0	0
58	2Z	1	Total 1	Mg 1	0	0
58	20	3	Total 3	Mg 3	0	0
58	21	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	23	2	Total Mg 2 2	0	0
58	25	4	Total Mg 4 4	0	0
58	26	1	Total Mg 1 1	0	0
58	27	2	Total Mg 2 2	0	0
58	28	3	Total Mg 3 3	0	0
58	2a	223	Total Mg 223 223	0	0
58	2d	2	Total Mg 2 2	0	0
58	2e	1	Total Mg 1 1	0	0
58	2f	2	Total Mg 2 2	0	0
58	2g	1	Total Mg 1 1	0	0
58	2j	1	Total Mg 1 1	0	0
58	2l	2	Total Mg 2 2	0	0
58	2q	2	Total Mg 2 2	0	0
58	2r	1	Total Mg 1 1	0	0
58	2t	1	Total Mg 1 1	0	0
58	2v	1	Total Mg 1 1	0	0
58	2w	2	Total Mg 2 2	0	0
58	2x	8	Total Mg 8 8	0	0

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

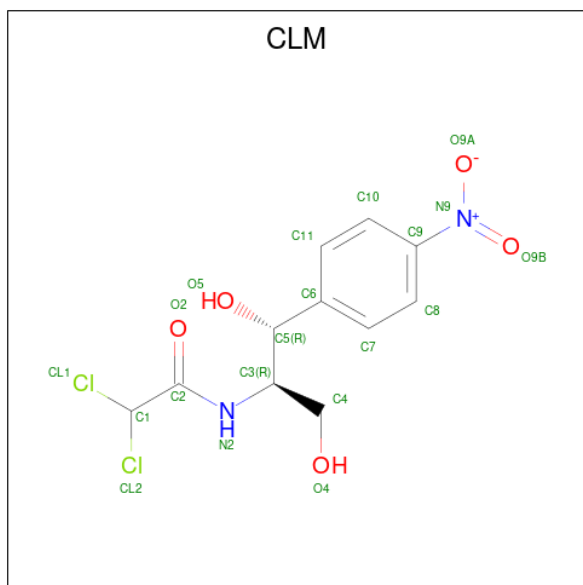
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	1A	1	Total K 1 1	0	0

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

- Molecule 60 is CHLORAMPHENICOL (three-letter code: CLM) (formula: $C_{11}H_{12}Cl_2N_2O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	1A	1	Total C Cl N O 20 11 2 2 5	0	0
60	2w	1	Total C Cl N O 20 11 2 2 5	0	0

- Molecule 61 is ZINC ION (three-letter code: ZN) (formula: Zn).

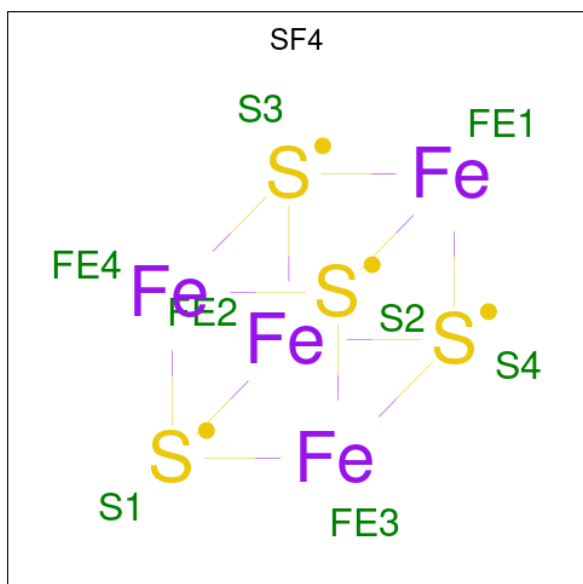
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1Y	1	Total Zn 1 1	0	0
61	14	1	Total Zn 1 1	0	0
61	15	1	Total Zn 1 1	0	0
61	16	1	Total Zn 1 1	0	0
61	19	1	Total Zn 1 1	0	0
61	1n	1	Total Zn 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2Y	1	Total	Zn	0	0
			1	1		
61	24	1	Total	Zn	0	0
			1	1		
61	25	1	Total	Zn	0	0
			1	1		
61	26	1	Total	Zn	0	0
			1	1		
61	29	1	Total	Zn	0	0
			1	1		
61	2n	1	Total	Zn	0	0
			1	1		

- Molecule 62 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
62	1d	1	Total	Fe	S	0	0
			8	4	4		
62	2d	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 63 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	1A	1977	Total	O	0	0
			1977	1977		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	1B	66	Total 66	O 66	0	0
63	1D	30	Total 30	O 30	0	0
63	1E	23	Total 23	O 23	0	0
63	1F	17	Total 17	O 17	0	0
63	1G	6	Total 6	O 6	0	0
63	1H	1	Total 1	O 1	0	0
63	1N	4	Total 4	O 4	0	0
63	1O	7	Total 7	O 7	0	0
63	1P	20	Total 20	O 20	0	0
63	1Q	7	Total 7	O 7	0	0
63	1R	9	Total 9	O 9	0	0
63	1S	5	Total 5	O 5	0	0
63	1T	8	Total 8	O 8	0	0
63	1U	11	Total 11	O 11	0	0
63	1V	9	Total 9	O 9	0	0
63	1W	7	Total 7	O 7	0	0
63	1X	7	Total 7	O 7	0	0
63	1Y	2	Total 2	O 2	0	0
63	10	11	Total 11	O 11	0	0
63	11	8	Total 8	O 8	0	0
63	12	3	Total 3	O 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	13	5	Total 5	O 5	0	0
63	14	1	Total 1	O 1	0	0
63	15	6	Total 6	O 6	0	0
63	16	2	Total 2	O 2	0	0
63	17	8	Total 8	O 8	0	0
63	18	12	Total 12	O 12	0	0
63	1a	263	Total 263	O 263	0	0
63	1b	1	Total 1	O 1	0	0
63	1d	1	Total 1	O 1	0	0
63	1e	1	Total 1	O 1	0	0
63	1f	1	Total 1	O 1	0	0
63	1g	1	Total 1	O 1	0	0
63	1l	6	Total 6	O 6	0	0
63	1m	2	Total 2	O 2	0	0
63	1n	1	Total 1	O 1	0	0
63	1o	1	Total 1	O 1	0	0
63	1q	3	Total 3	O 3	0	0
63	1u	1	Total 1	O 1	0	0
63	1v	3	Total 3	O 3	0	0
63	1w	5	Total 5	O 5	0	0
63	1x	11	Total 11	O 11	0	0

Continued on next page...

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	1y	1	Total 1	O 1	0	0
63	2A	1074	Total 1074	O 1074	0	0
63	2B	18	Total 18	O 18	0	0
63	2D	22	Total 22	O 22	0	0
63	2E	13	Total 13	O 13	0	0
63	2F	12	Total 12	O 12	0	0
63	2I	2	Total 2	O 2	0	0
63	2N	1	Total 1	O 1	0	0
63	2O	3	Total 3	O 3	0	0
63	2P	11	Total 11	O 11	0	0
63	2Q	2	Total 2	O 2	0	0
63	2R	3	Total 3	O 3	0	0
63	2T	2	Total 2	O 2	0	0
63	2U	3	Total 3	O 3	0	0
63	2W	2	Total 2	O 2	0	0
63	2X	5	Total 5	O 5	0	0
63	2Y	1	Total 1	O 1	0	0
63	2Z	1	Total 1	O 1	0	0
63	20	3	Total 3	O 3	0	0
63	21	5	Total 5	O 5	0	0
63	23	1	Total 1	O 1	0	0

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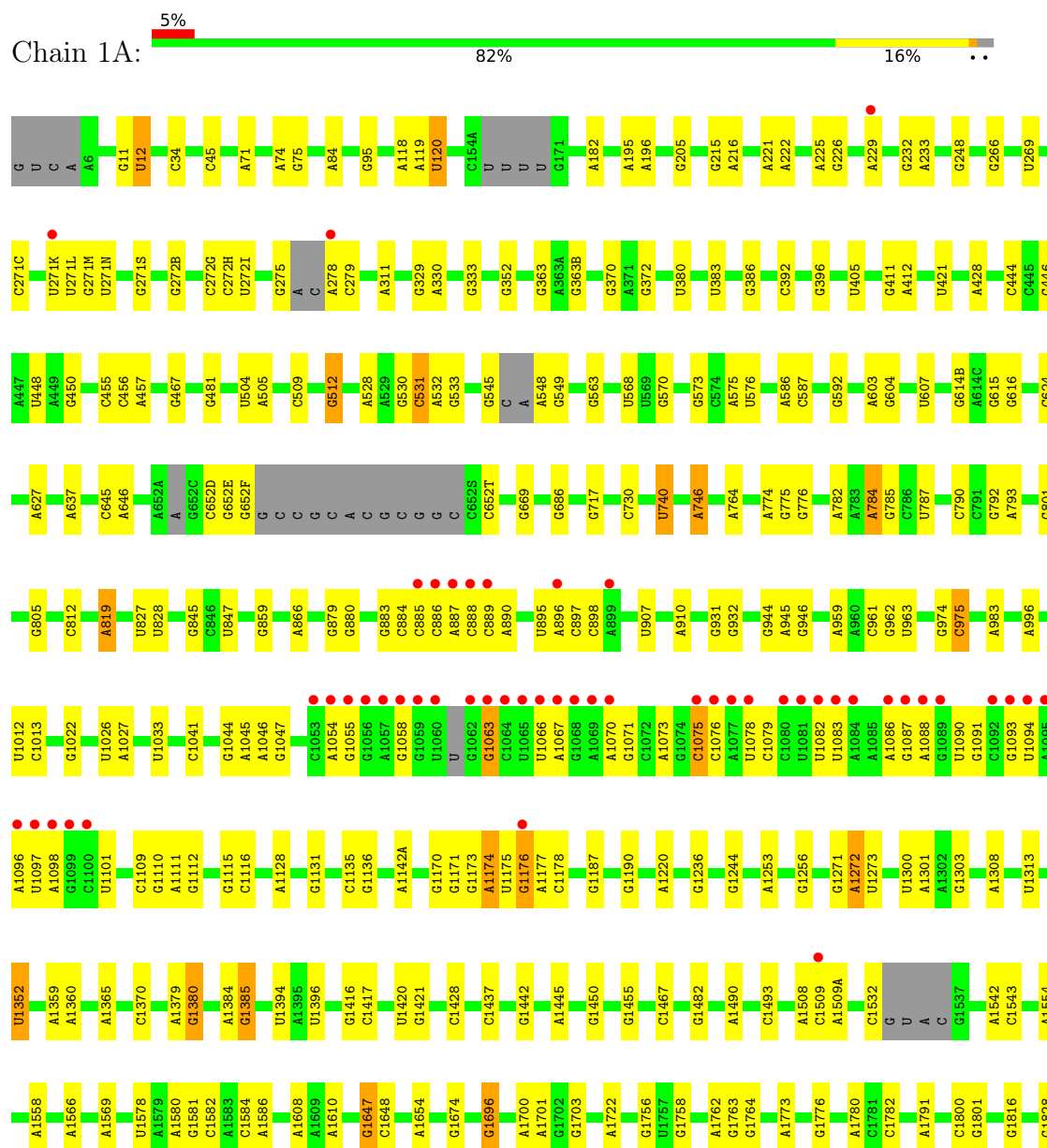
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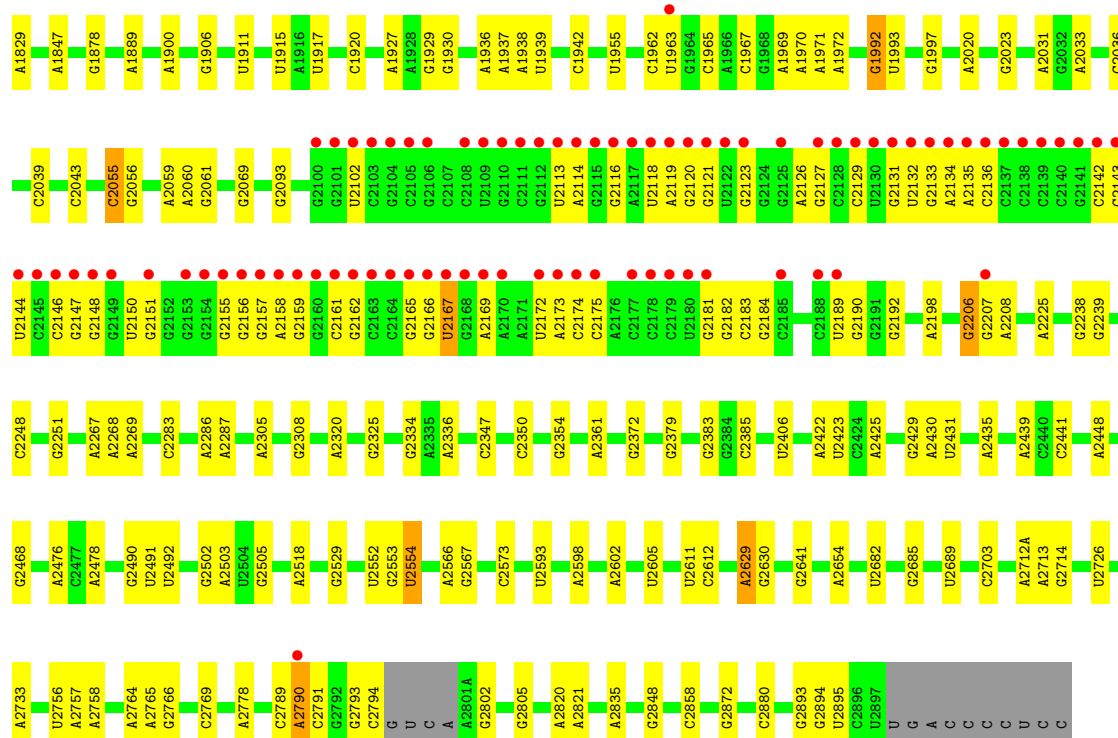
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	27	2	Total 2	O 2	0	0
63	28	6	Total 6	O 6	0	0
63	29	1	Total 1	O 1	0	0
63	2a	245	Total 245	O 245	0	0
63	2d	2	Total 2	O 2	0	0
63	2j	1	Total 1	O 1	0	0
63	2l	3	Total 3	O 3	0	0
63	2o	1	Total 1	O 1	0	0
63	2p	2	Total 2	O 2	0	0
63	2q	1	Total 1	O 1	0	0
63	2r	1	Total 1	O 1	0	0
63	2t	2	Total 2	O 2	0	0
63	2v	1	Total 1	O 1	0	0
63	2w	2	Total 2	O 2	0	0
63	2x	6	Total 6	O 6	0	0
63	2z	1	Total 1	O 1	0	0

3 Residue-property plots [i](#)

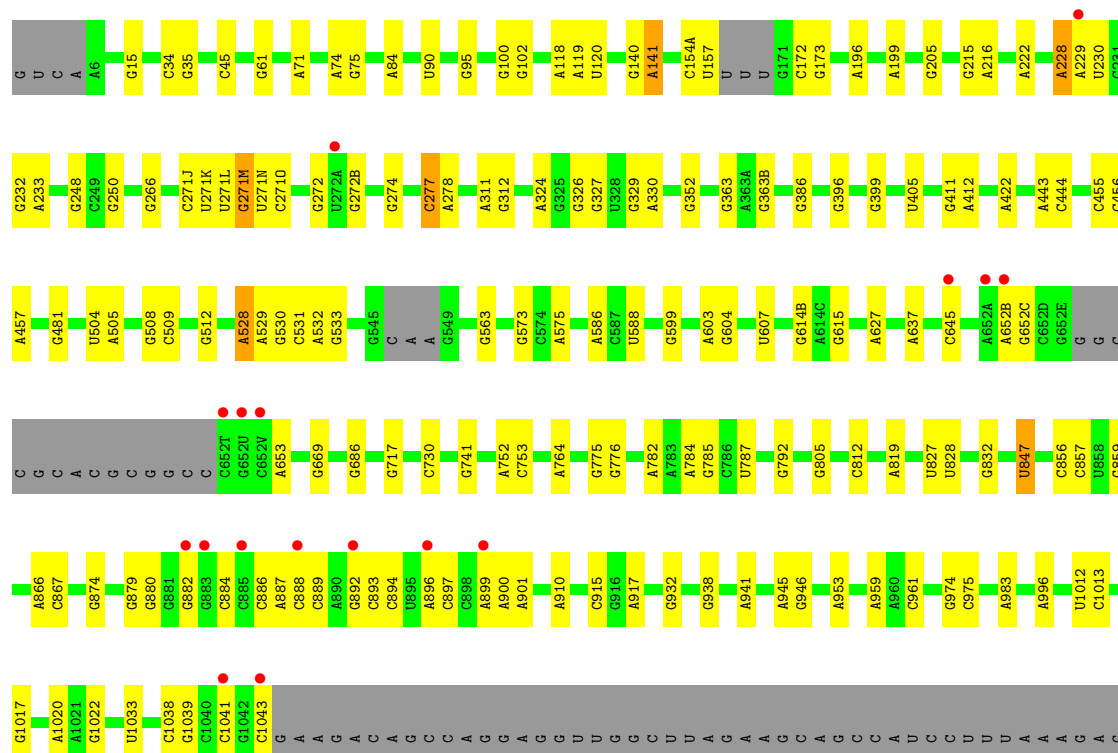
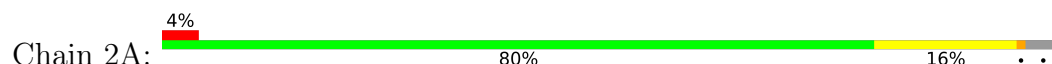
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: 23S Ribosomal RNA



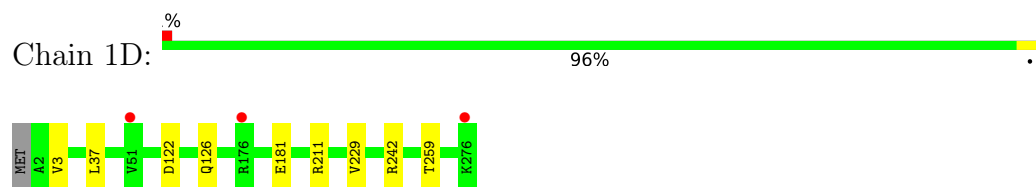


- Molecule 1: 23S Ribosomal RNA

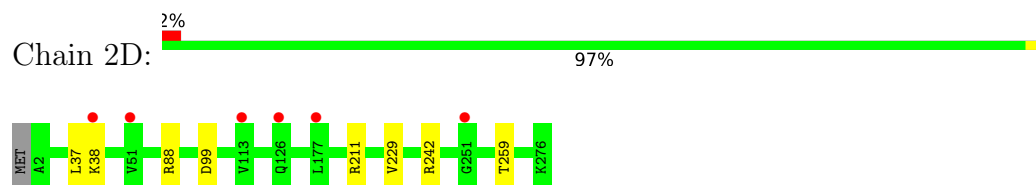




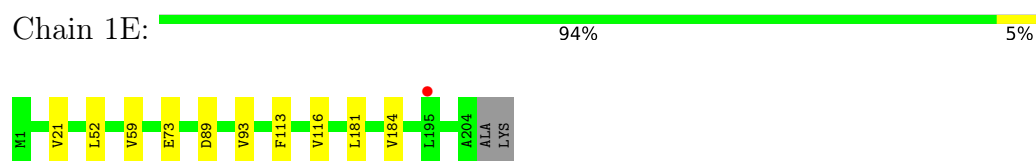
- Molecule 3: 50S ribosomal protein L2



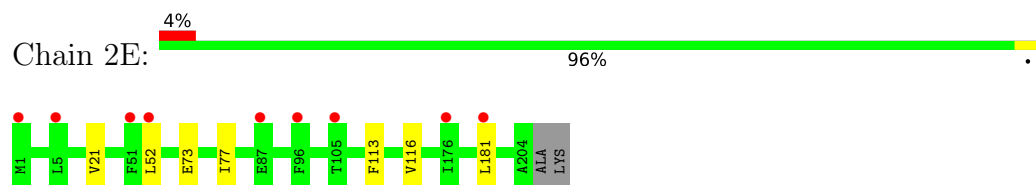
- Molecule 3: 50S ribosomal protein L2



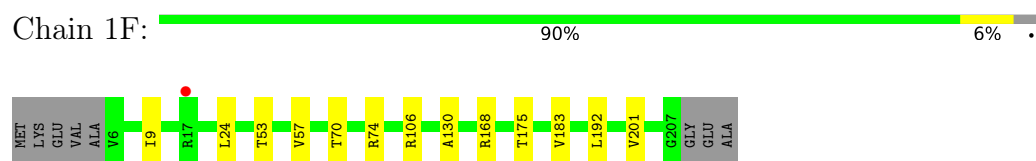
- Molecule 4: 50S ribosomal protein L3



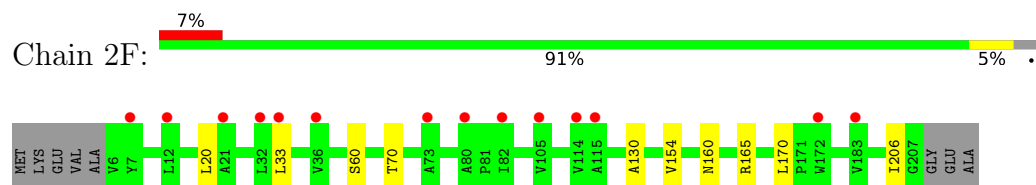
- Molecule 4: 50S ribosomal protein L3



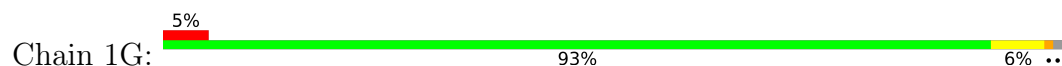
- Molecule 5: 50S ribosomal protein L4

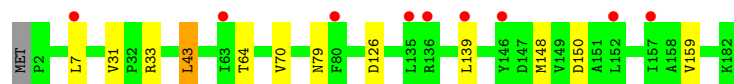


- Molecule 5: 50S ribosomal protein L4

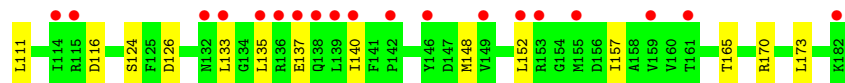
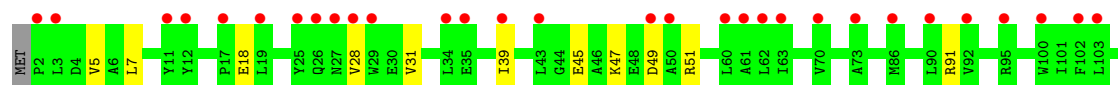
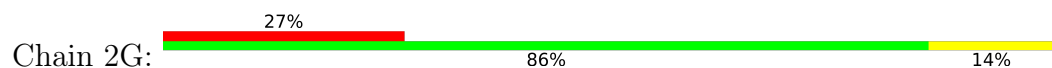


- Molecule 6: 50S ribosomal protein L5





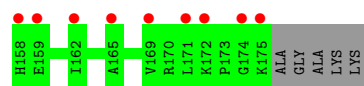
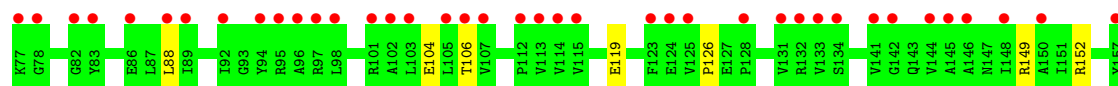
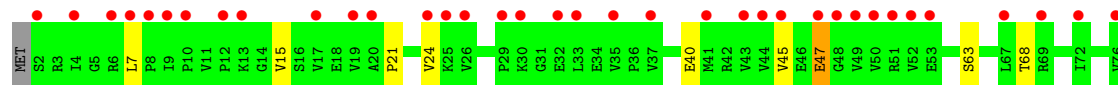
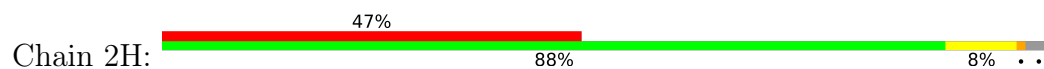
- Molecule 6: 50S ribosomal protein L5



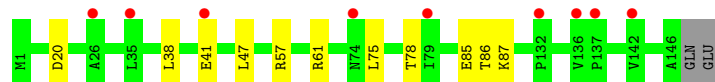
- Molecule 7: 50S ribosomal protein L6



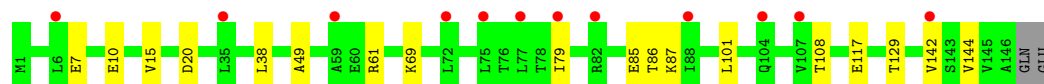
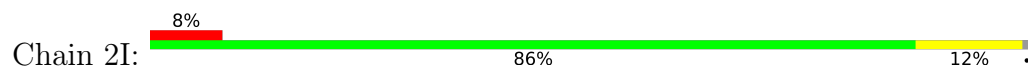
- Molecule 7: 50S ribosomal protein L6



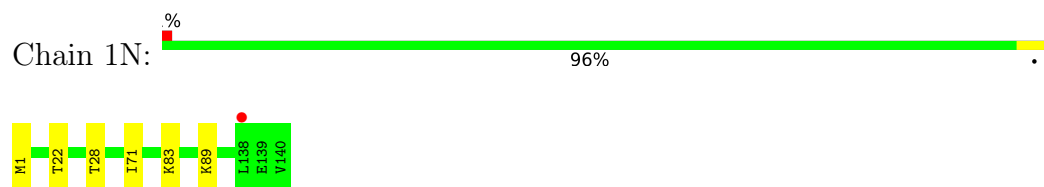
- Molecule 8: 50S ribosomal protein L9



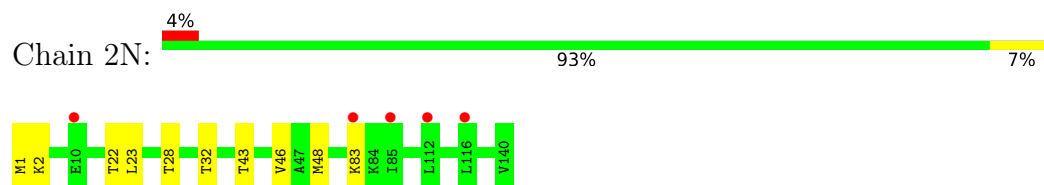
- Molecule 8: 50S ribosomal protein L9



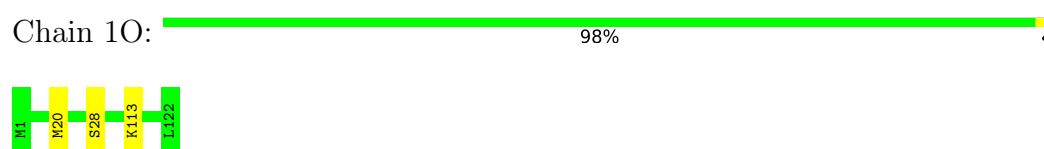
- Molecule 9: 50S ribosomal protein L13



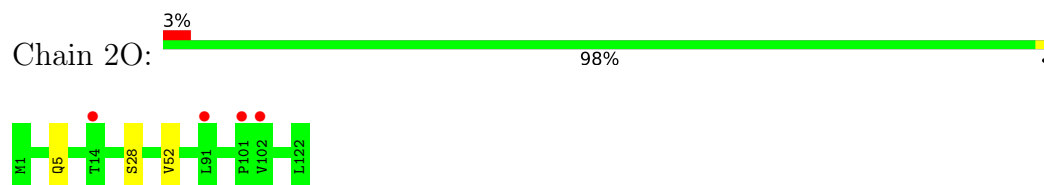
- Molecule 9: 50S ribosomal protein L13



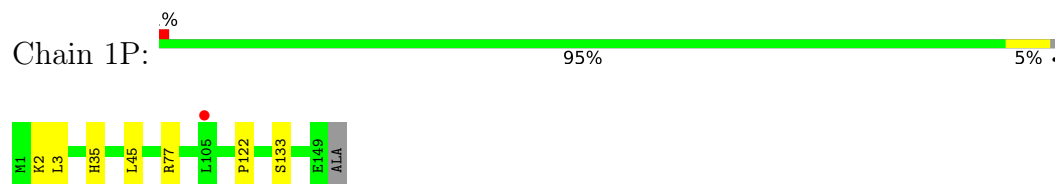
- Molecule 10: 50S ribosomal protein L14



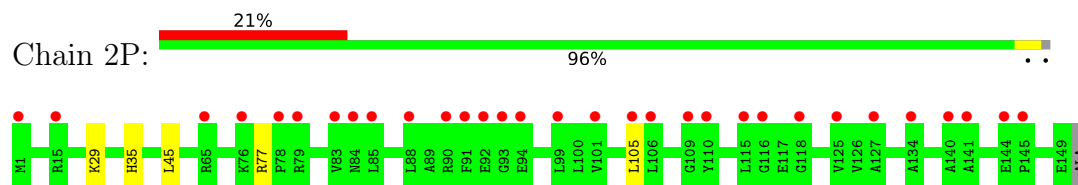
- Molecule 10: 50S ribosomal protein L14



- Molecule 11: 50S ribosomal protein L15



- Molecule 11: 50S ribosomal protein L15

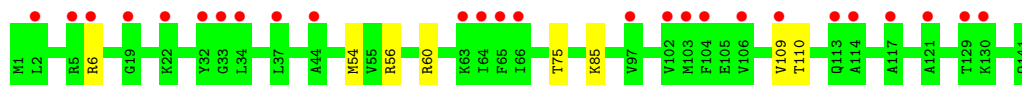


- Molecule 12: 50S ribosomal protein L16





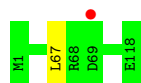
- Molecule 12: 50S ribosomal protein L16



- Molecule 13: 50S ribosomal protein L17



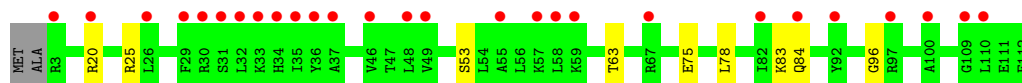
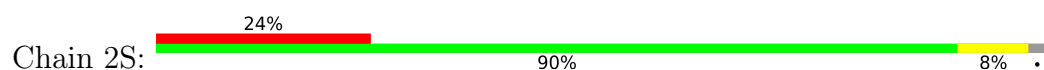
- Molecule 13: 50S ribosomal protein L17



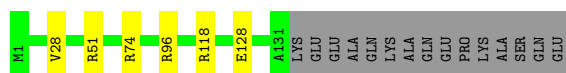
- Molecule 14: 50S ribosomal protein L18



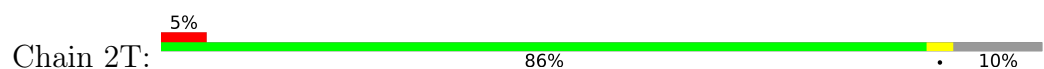
- Molecule 14: 50S ribosomal protein L18



- Molecule 15: 50S ribosomal protein L19



- Molecule 15: 50S ribosomal protein L19

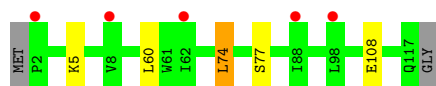




- Molecule 16: 50S ribosomal protein L20



- Molecule 16: 50S ribosomal protein L20



- Molecule 17: 50S ribosomal protein L21



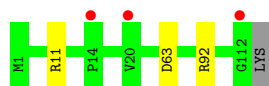
- Molecule 17: 50S ribosomal protein L21



- Molecule 18: 50S ribosomal protein L22



- Molecule 18: 50S ribosomal protein L22



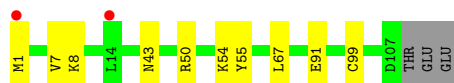
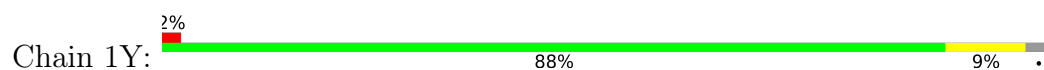
- Molecule 19: 50S ribosomal protein L23



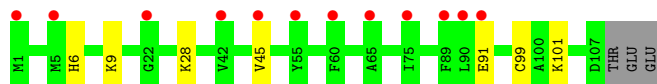
- Molecule 19: 50S ribosomal protein L23



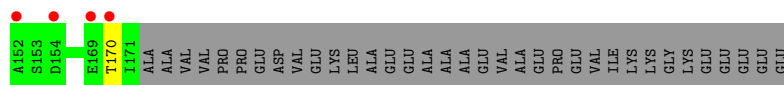
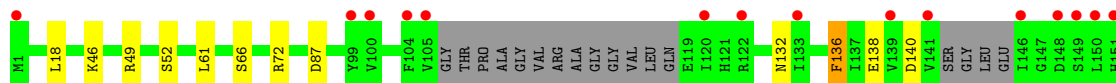
- Molecule 20: 50S ribosomal protein L24



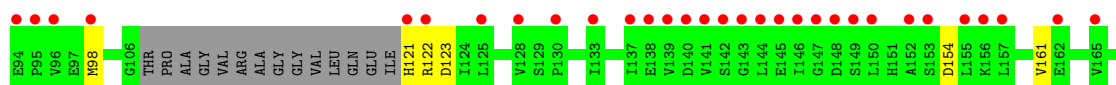
- Molecule 20: 50S ribosomal protein L24

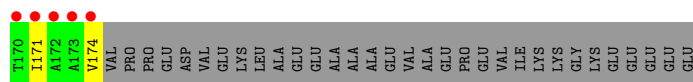


- Molecule 21: 50S ribosomal protein L25

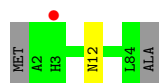


- Molecule 21: 50S ribosomal protein L25

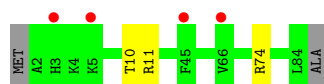




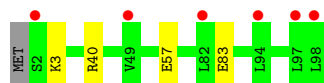
- Molecule 22: 50S ribosomal protein L27



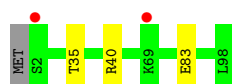
- Molecule 22: 50S ribosomal protein L27



- Molecule 23: 50S ribosomal protein L28



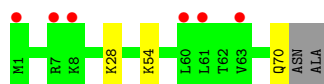
- Molecule 23: 50S ribosomal protein L28



- Molecule 24: 50S ribosomal protein L29



- Molecule 24: 50S ribosomal protein L29



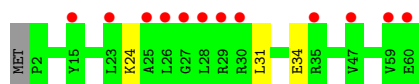
- Molecule 25: 50S ribosomal protein L30

Chain 13:  95% . .




- Molecule 25: 50S ribosomal protein L30

Chain 23:  20% 93% 5% .




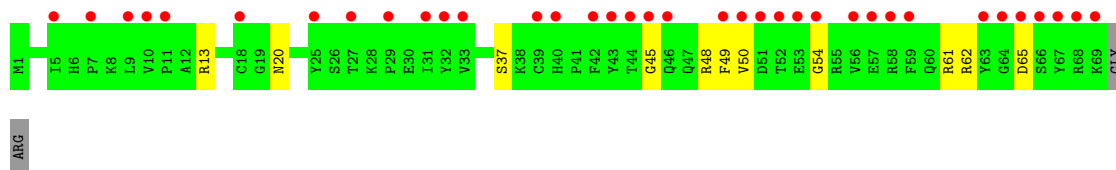
- Molecule 26: 50S ribosomal protein L31

Chain 14:  21% 86% 8% . .

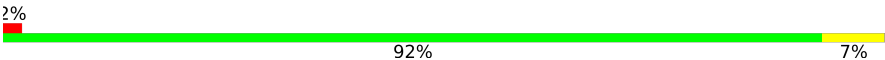


- Molecule 26: 50S ribosomal protein L31

Chain 24:  51% 82% 15% .



- Molecule 27: 50S ribosomal protein L32

Chain 15:  2% 92% 7% .



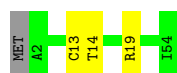
- Molecule 27: 50S ribosomal protein L32

Chain 25:  3% 93% 5% .

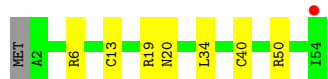
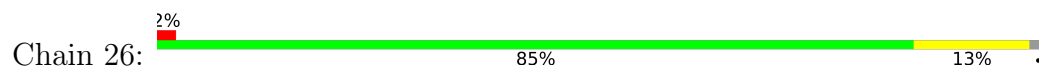


- Molecule 28: 50S ribosomal protein L33

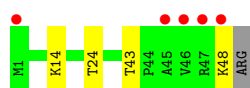
Chain 16:  93% 6% .



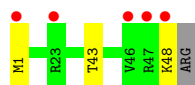
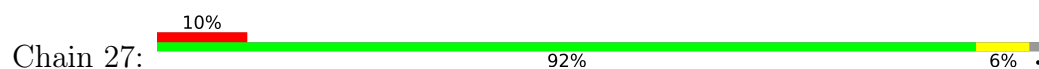
- Molecule 28: 50S ribosomal protein L33



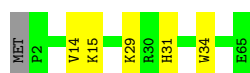
- Molecule 29: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L34



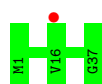
- Molecule 30: 50S ribosomal protein L35



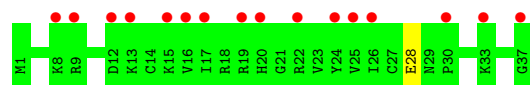
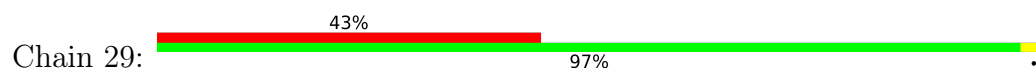
- Molecule 30: 50S ribosomal protein L35



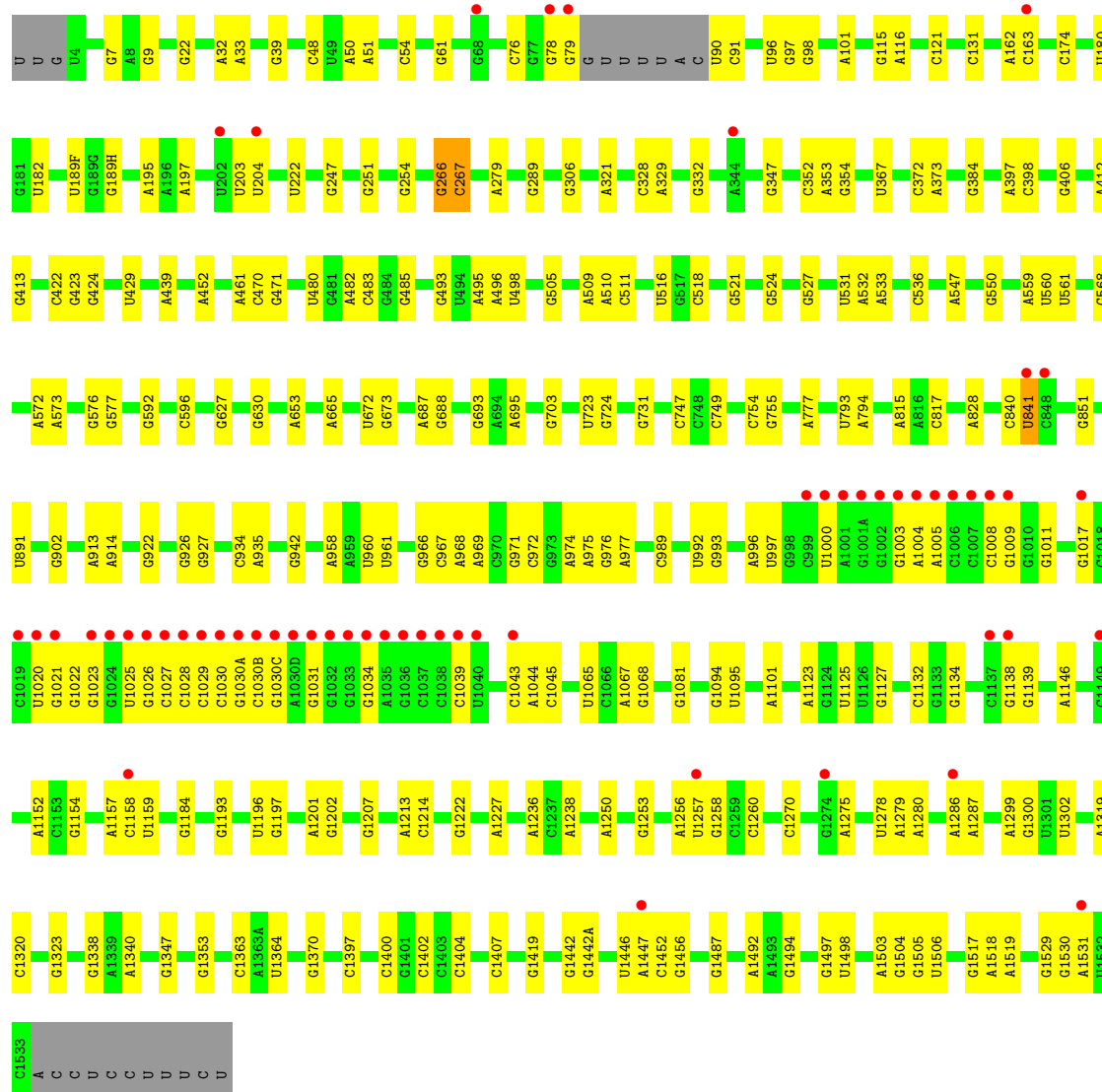
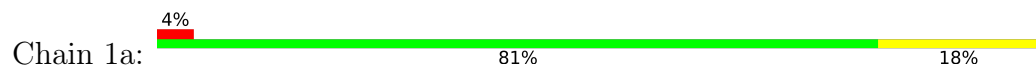
- Molecule 31: 50S ribosomal protein L36



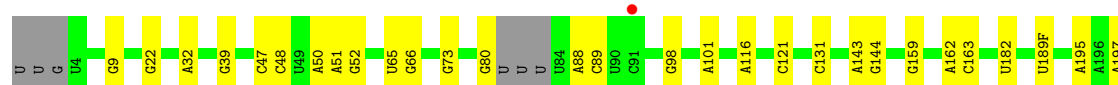
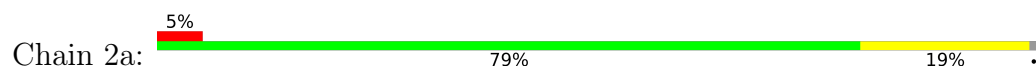
- Molecule 31: 50S ribosomal protein L36

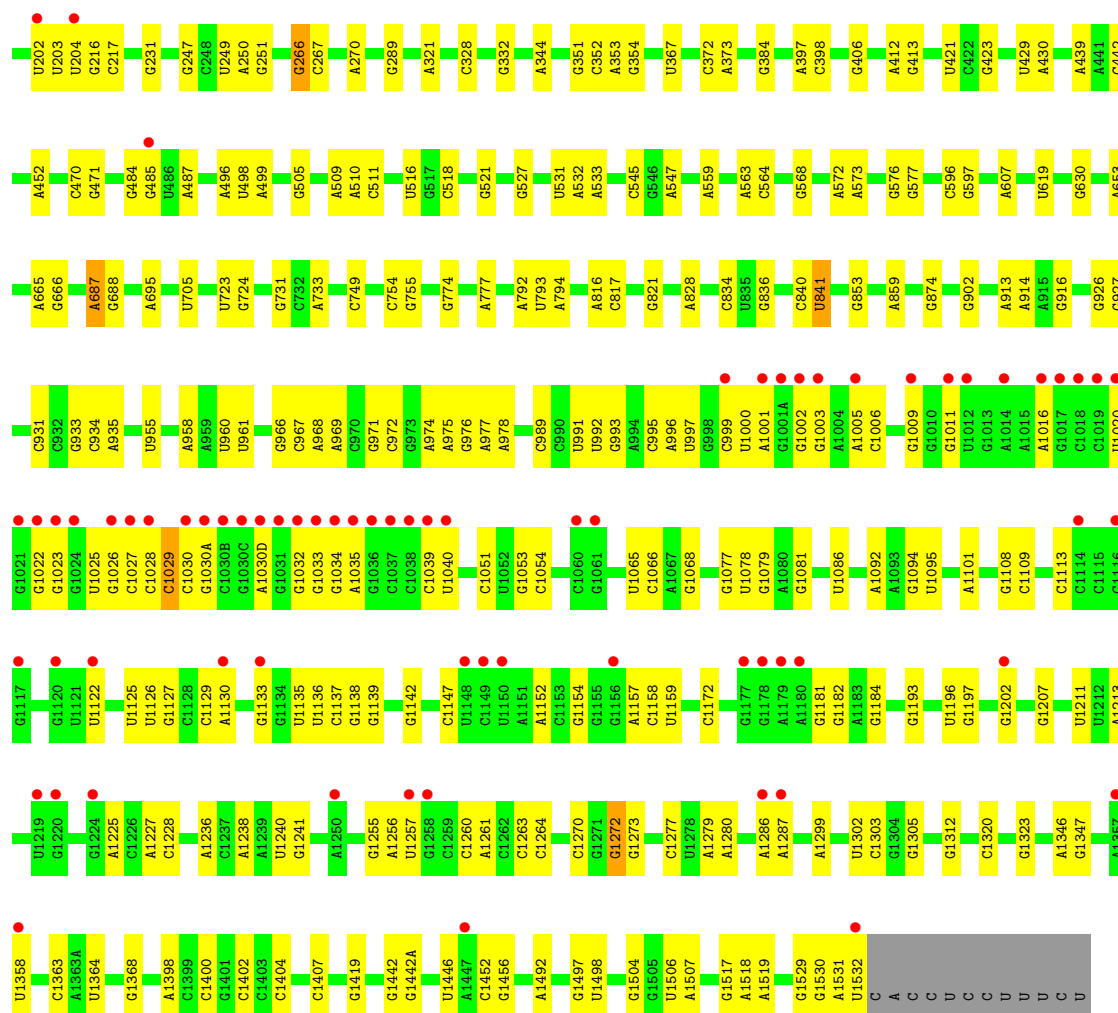


• Molecule 32: 16S Ribosomal RNA

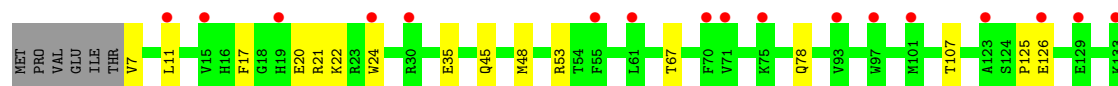
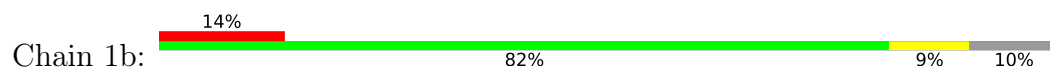


• Molecule 32: 16S Ribosomal RNA

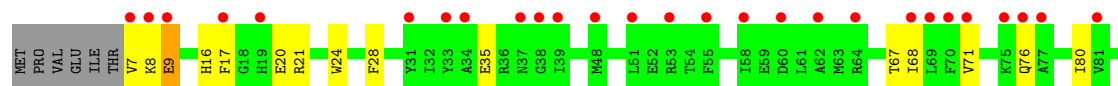
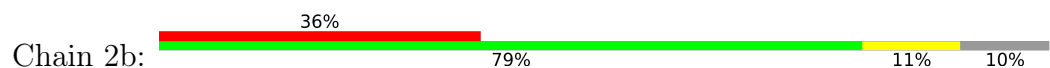


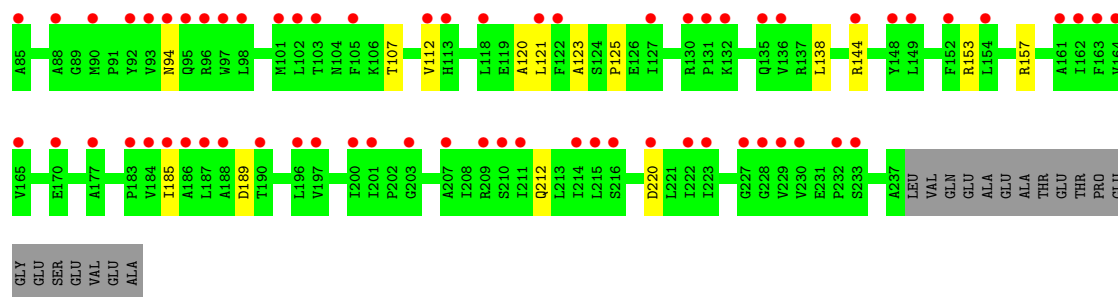


• Molecule 33: 30S ribosomal protein S2

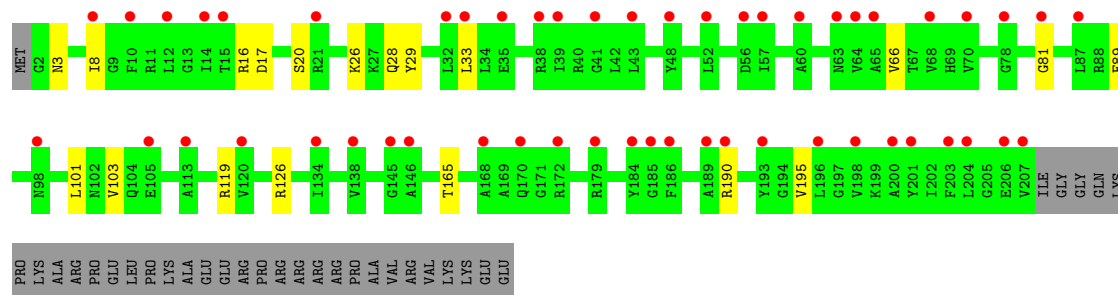
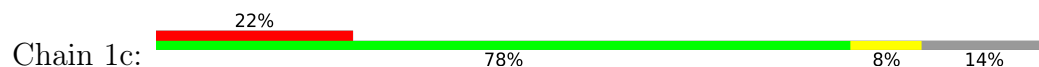


• Molecule 33: 30S ribosomal protein S2

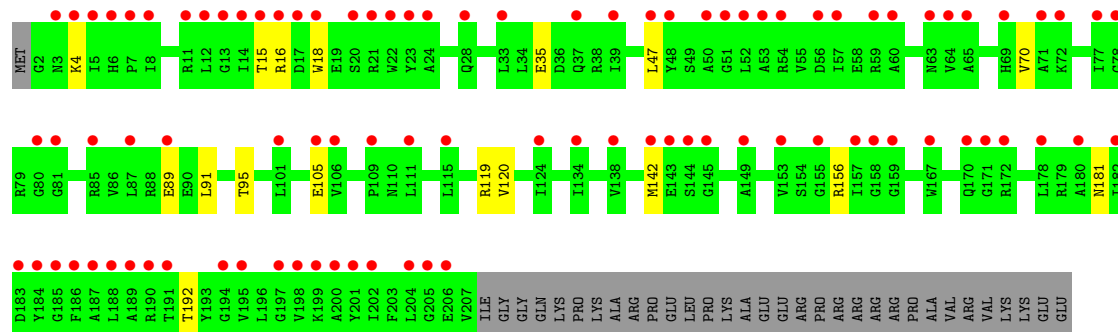
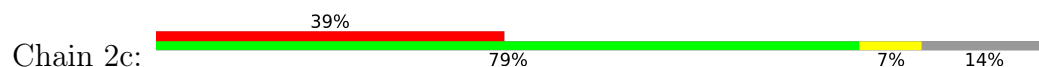




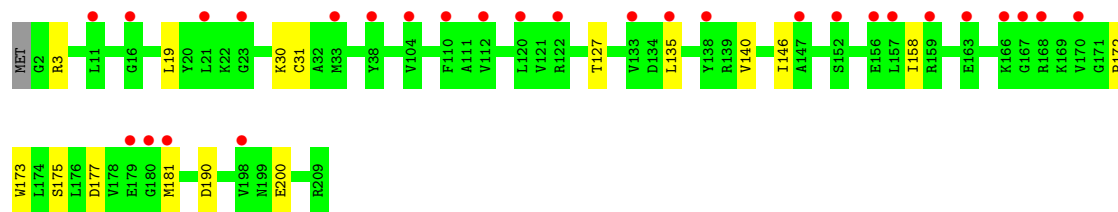
• Molecule 34: 30S ribosomal protein S3



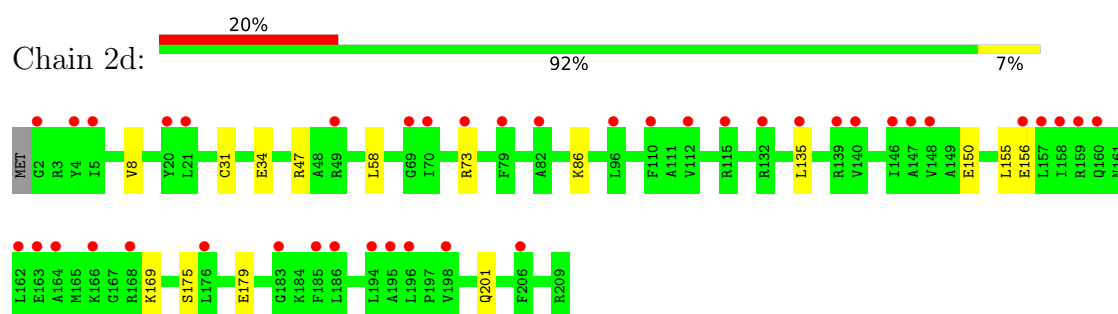
• Molecule 34: 30S ribosomal protein S3



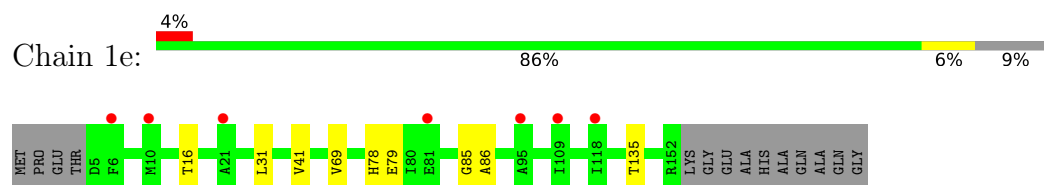
• Molecule 35: 30S ribosomal protein S4



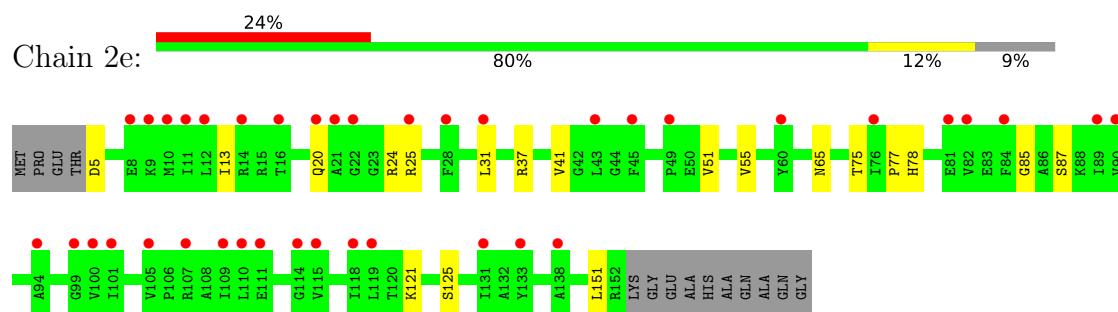
• Molecule 35: 30S ribosomal protein S4



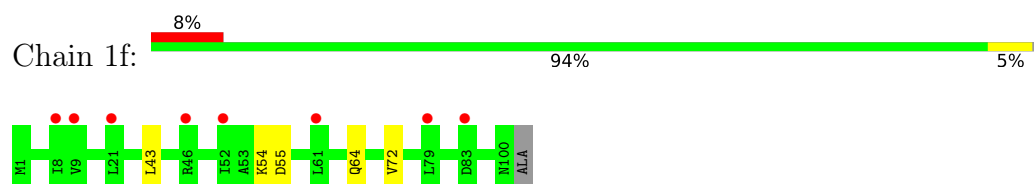
- Molecule 36: 30S ribosomal protein S5



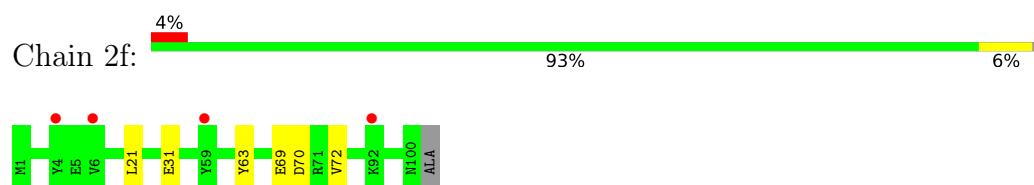
- Molecule 36: 30S ribosomal protein S5



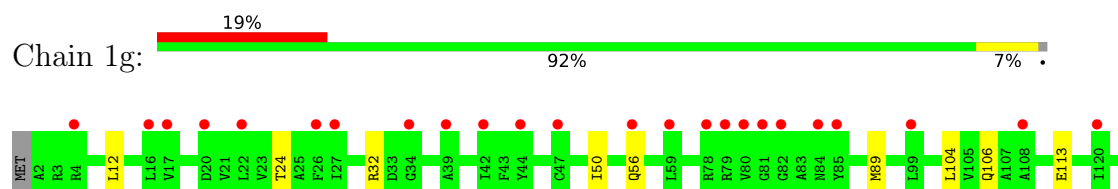
- Molecule 37: 30S ribosomal protein S6



- Molecule 37: 30S ribosomal protein S6

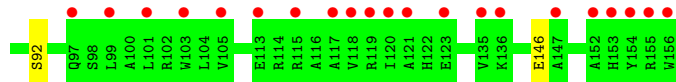
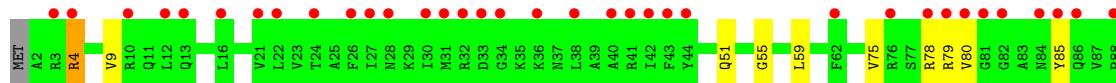
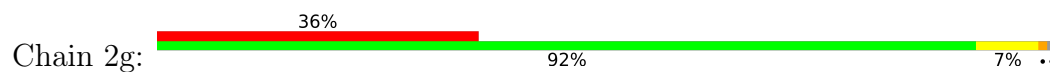


- Molecule 38: 30S ribosomal protein S7

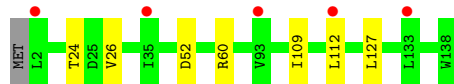




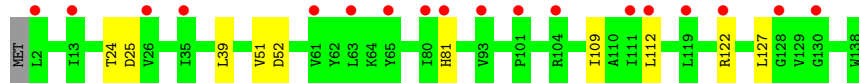
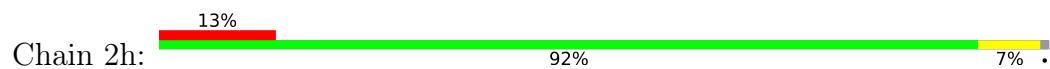
- Molecule 38: 30S ribosomal protein S7



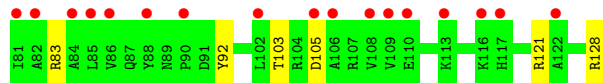
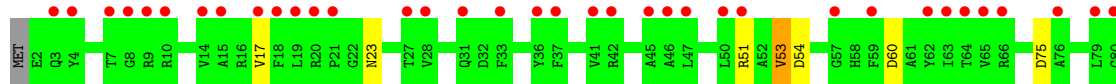
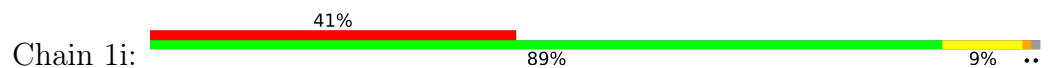
- Molecule 39: 30S ribosomal protein S8



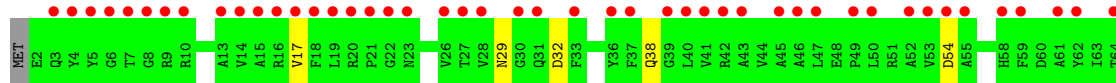
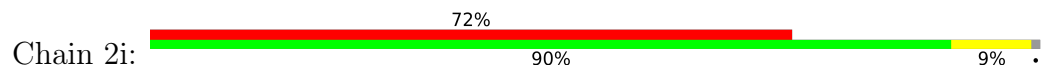
- Molecule 39: 30S ribosomal protein S8

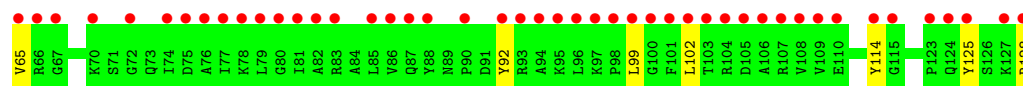


- Molecule 40: 30S ribosomal protein S9

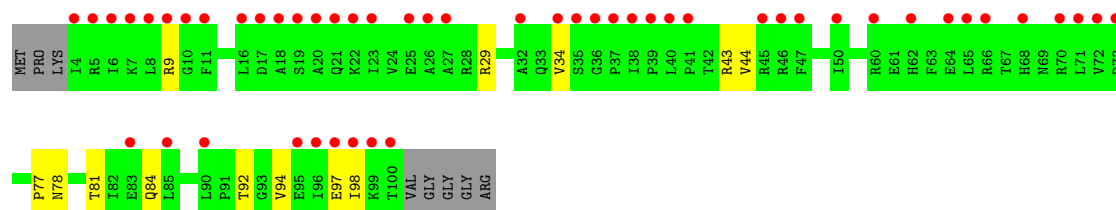
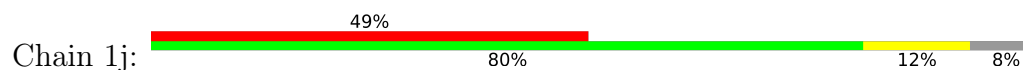


- Molecule 40: 30S ribosomal protein S9

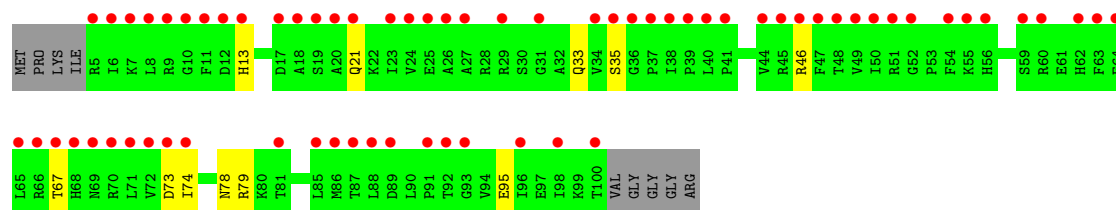
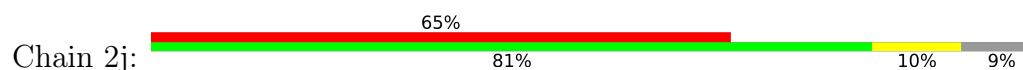




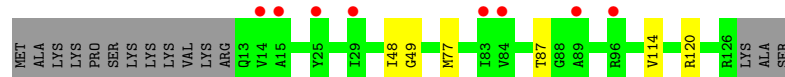
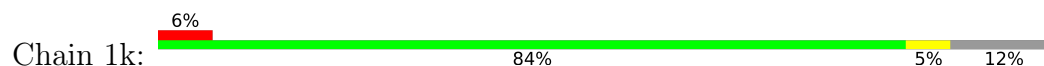
- Molecule 41: 30S ribosomal protein S10



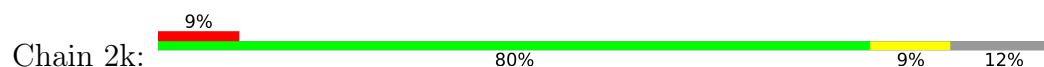
- Molecule 41: 30S ribosomal protein S10



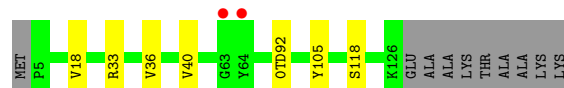
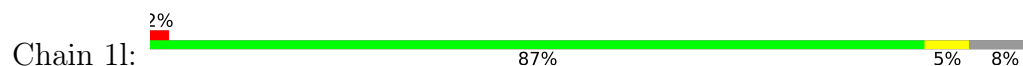
- Molecule 42: 30S ribosomal protein S11



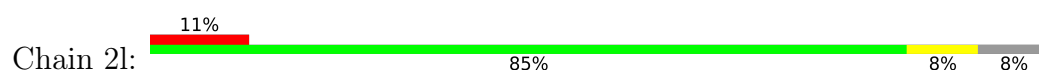
- Molecule 42: 30S ribosomal protein S11



- Molecule 43: 30S ribosomal protein S12



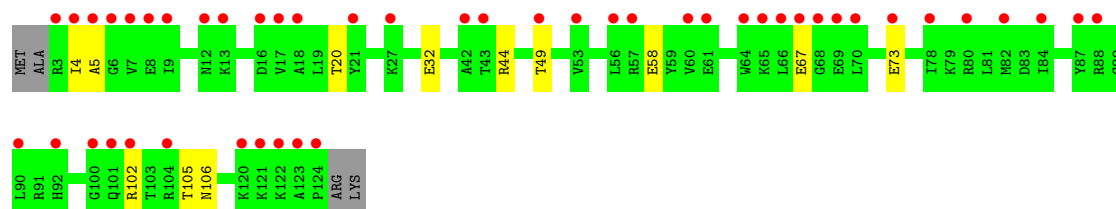
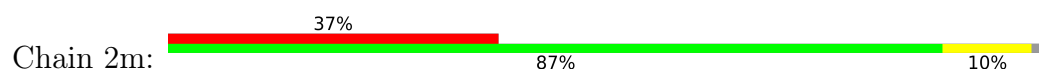
- Molecule 43: 30S ribosomal protein S12



- Molecule 44: 30S ribosomal protein S13



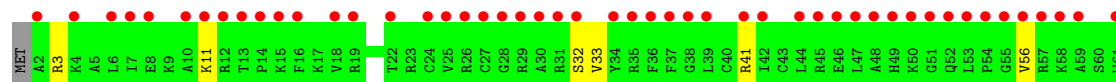
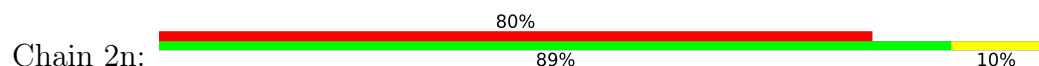
- Molecule 44: 30S ribosomal protein S13



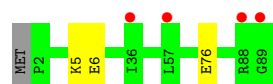
- Molecule 45: 30S ribosomal protein S14 type Z



- Molecule 45: 30S ribosomal protein S14 type Z

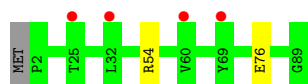


- Molecule 46: 30S ribosomal protein S15

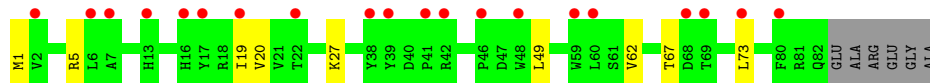
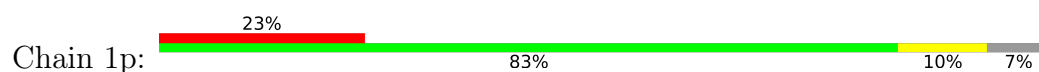


- Molecule 46: 30S ribosomal protein S15

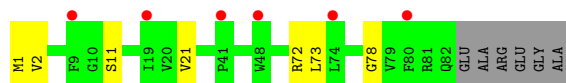
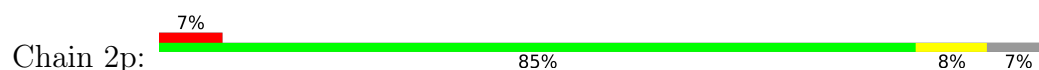




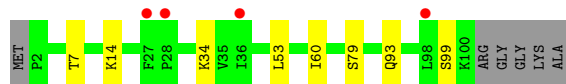
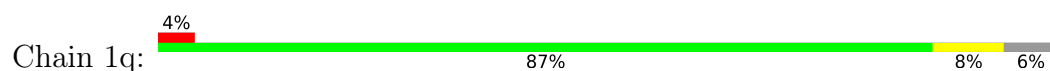
- Molecule 47: 30S ribosomal protein S16



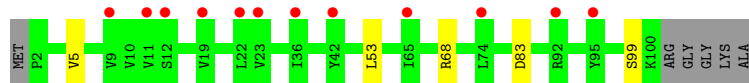
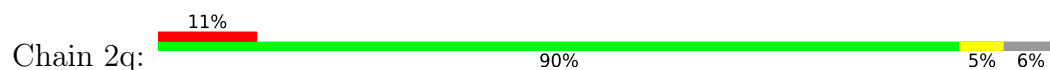
- Molecule 47: 30S ribosomal protein S16



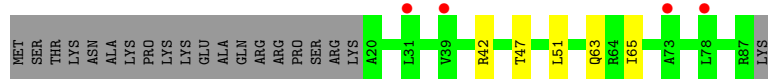
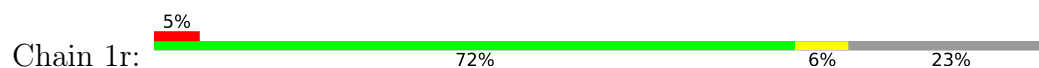
- Molecule 48: 30S ribosomal protein S17



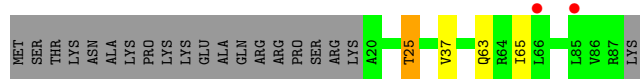
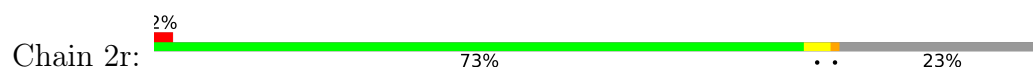
- Molecule 48: 30S ribosomal protein S17



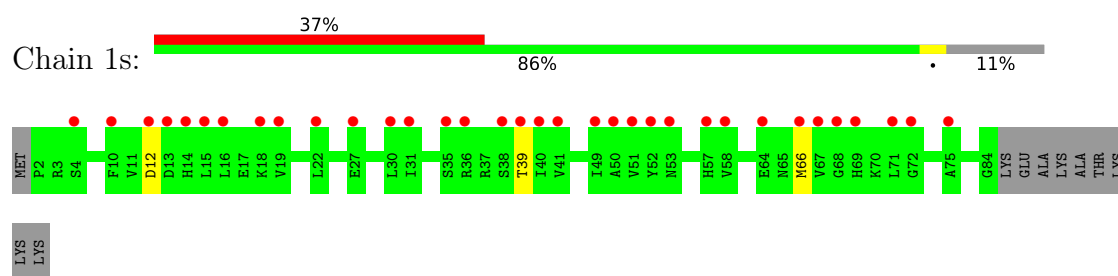
- Molecule 49: 30S ribosomal protein S18



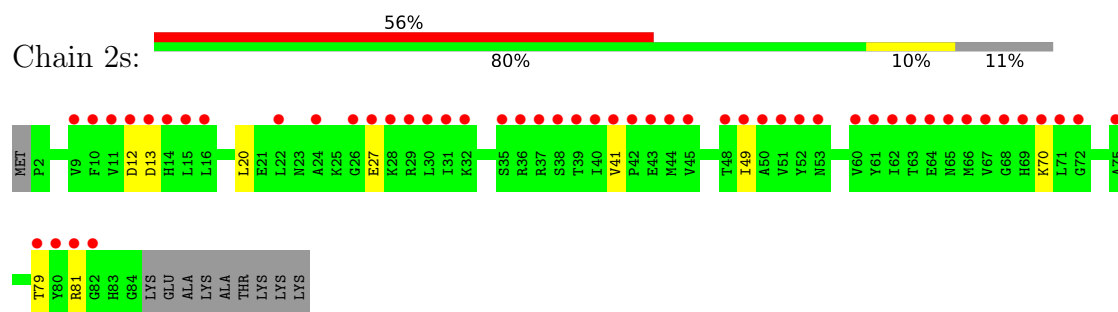
- Molecule 49: 30S ribosomal protein S18



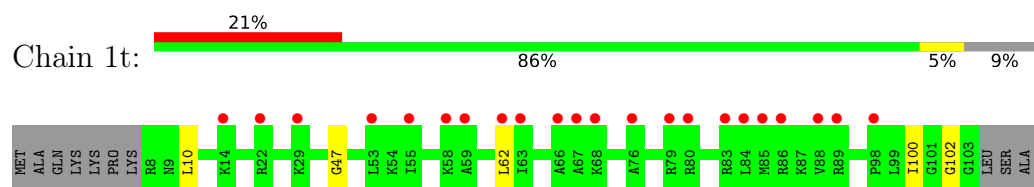
- Molecule 50: 30S ribosomal protein S19



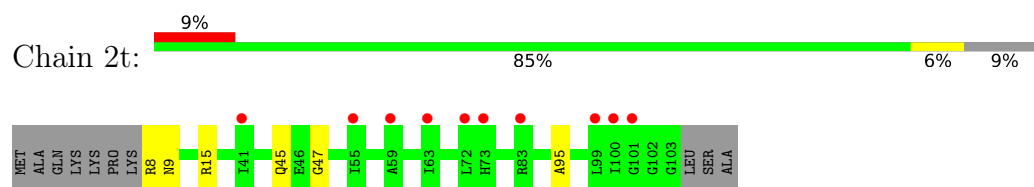
- Molecule 50: 30S ribosomal protein S19



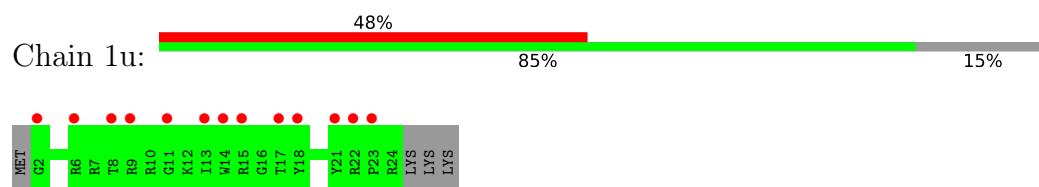
- Molecule 51: 30S ribosomal protein S20



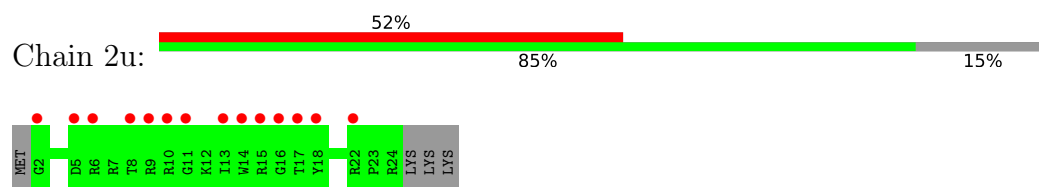
- Molecule 51: 30S ribosomal protein S20



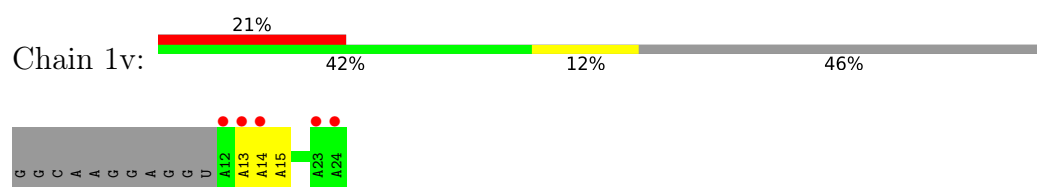
- Molecule 52: 30S ribosomal protein Thx



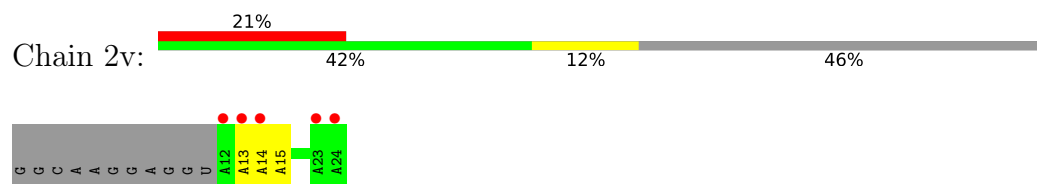
- Molecule 52: 30S ribosomal protein Thx



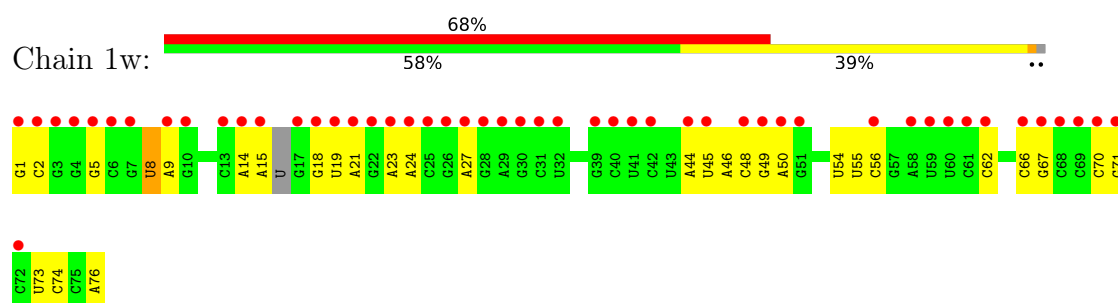
- Molecule 53: MG-mRNA



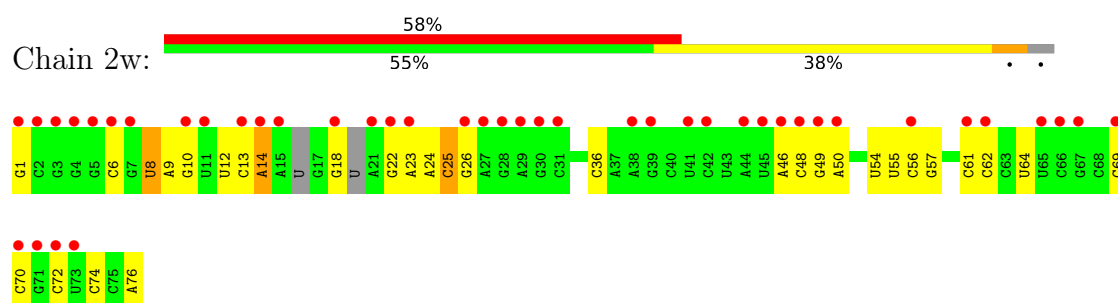
- Molecule 53: MG-mRNA



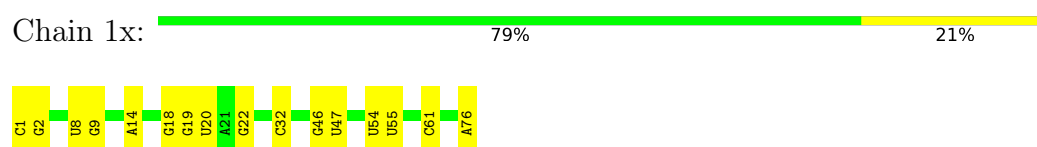
- Molecule 54: A-site Aminoacyl-tRNA Gly-NH-tRNAgly



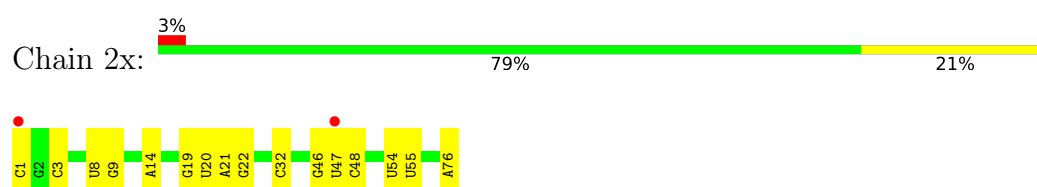
- Molecule 54: A-site Aminoacyl-tRNA Gly-NH-tRNAgly



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



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



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

Chain 1z:  100%


There are no outlier residues recorded for this chain.

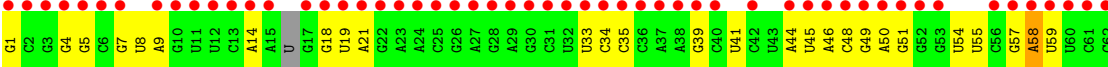
- Molecule 56: P-site Peptidyl-tRNA fMAC-NH-tRNA^{met} Peptide-part

Chain 2z:  67% 33%

 M1
A2
C3

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


Chain 1y:  55% 42% 86% ..


 G1 C2 C3 C4 C5 C6 C7 C8 C9 C10 C11 C12 C13 C14 A15 U G17 G18 U19 U21 A21 G22 A23 A24 A25 C26 G27 A28 G29 A30 C31 C32 U33 U34 C35 C36 A37 A38 A39 C40 U41 C42 U43 A44 U45 A46 C48 C49 A50 G51 G52 G53 U54 U55 C56 G57 A58 U59 U60 C61 C62

 C63 U64 U65 C66 C67 C68 C69 C70 G71 C72 U73 C74 C75 A76

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

Chain 2y:  51% 39% 93% 8%

 G1 C2 C3 C4 C5 C6 C7 C8 C9 C10 C11 C12 C13 C14 A15 U G17 G18 U19 U21 A21 G22 A23 A24 A25 C26 G27 A28 G29 A30 C31 C32 U33 U34 C35 C36 A37 A38 A39 C40 U41 C42 U43 A44 U45 A46 C48 C49 A50 G51 G52 G53 U54 U55 C56 G57 A58 U59 U60 C61 C62

 C63 U64 U65 C66 C67 C68 C69 C70 G71 C72 U73 C74 C75 A76

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.93Å 451.24Å 622.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	125.00 – 2.55 174.03 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.5 (125.00-2.55) 99.5 (174.03-2.55)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 2.55Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.213 , 0.256 0.214 , 0.256	Depositor DCC
R_{free} test set	94560 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	61.7	Xtriage
Anisotropy	0.169	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 52.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	299751	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.65% 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: SF4, ZN, 2MA, 0TD, PSU, OMC, OMU, UR3, 4SU, G7M, 2MG, OMG, 5MU, M2G, K, FME, CLM, MA6, 8AN, 5MC, 4OC, L3X, MG

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	0.51	0/69011	0.95	90/107720 (0.1%)
1	2A	0.38	0/67295	0.85	34/105042 (0.0%)
2	1B	0.43	1/2882 (0.0%)	0.82	0/4494
2	2B	0.38	1/2879 (0.0%)	0.83	2/4487 (0.0%)
3	1D	0.35	0/2186	0.56	0/2944
3	2D	0.30	0/2186	0.50	0/2944
4	1E	0.34	0/1592	0.53	0/2149
4	2E	0.29	0/1592	0.50	0/2149
5	1F	0.33	0/1618	0.53	0/2191
5	2F	0.29	0/1614	0.49	0/2186
6	1G	0.29	0/1448	0.49	0/1957
6	2G	0.29	0/1453	0.48	0/1963
7	1H	0.31	0/1356	0.49	0/1834
7	2H	0.29	0/1356	0.46	0/1834
8	1I	0.29	0/1112	0.51	0/1514
8	2I	0.26	0/1079	0.47	0/1475
9	1N	0.33	0/1144	0.49	0/1543
9	2N	0.28	0/1144	0.45	0/1543
10	1O	0.33	0/943	0.53	0/1269
10	2O	0.30	0/943	0.51	0/1269
11	1P	0.32	0/1152	0.57	0/1533
11	2P	0.31	0/1152	0.52	0/1533
12	1Q	0.35	0/1143	0.54	0/1527
12	2Q	0.29	0/1143	0.46	0/1527
13	1R	0.32	0/982	0.51	0/1312
13	2R	0.27	0/982	0.49	0/1312
14	1S	0.32	0/883	0.51	0/1176
14	2S	0.30	0/880	0.49	0/1172
15	1T	0.31	0/1105	0.50	0/1477
15	2T	0.28	0/1097	0.47	0/1468
16	1U	0.34	0/977	0.49	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.27	0/977	0.44	1/1301 (0.1%)
17	1V	0.33	0/782	0.53	0/1049
17	2V	0.29	0/782	0.48	0/1049
18	1W	0.34	0/897	0.53	0/1205
18	2W	0.29	0/897	0.48	0/1205
19	1X	0.37	0/764	0.57	0/1025
19	2X	0.30	0/764	0.51	0/1025
20	1Y	0.33	0/819	0.53	0/1095
20	2Y	0.31	0/819	0.50	0/1095
21	1Z	0.31	0/1267	0.52	0/1717
21	2Z	0.30	0/1299	0.47	0/1763
22	10	0.34	0/662	0.58	1/881 (0.1%)
22	20	0.31	0/662	0.49	0/881
23	11	0.33	0/762	0.53	0/1014
23	21	0.30	0/762	0.50	0/1014
24	12	0.31	0/590	0.44	0/781
24	22	0.27	0/590	0.41	0/781
25	13	0.31	0/474	0.51	0/635
25	23	0.27	0/469	0.44	0/630
26	14	0.32	0/565	0.56	0/761
26	24	0.32	0/545	0.54	0/737
27	15	0.31	0/469	0.53	0/635
27	25	0.29	0/469	0.51	0/635
28	16	0.35	0/460	0.53	0/613
28	26	0.26	0/456	0.48	0/608
29	17	0.35	0/426	0.54	0/561
29	27	0.30	0/426	0.49	0/561
30	18	0.31	0/525	0.53	0/691
30	28	0.29	0/525	0.48	0/691
31	19	0.36	0/310	0.53	0/407
31	29	0.30	0/310	0.52	0/407
32	1a	0.35	0/35795	0.85	22/55864 (0.0%)
32	2a	0.34	2/35886 (0.0%)	0.86	37/56005 (0.1%)
33	1b	0.28	0/1881	0.48	0/2542
33	2b	0.29	0/1860	0.48	0/2518
34	1c	0.28	0/1572	0.45	0/2126
34	2c	0.29	0/1566	0.48	0/2119
35	1d	0.28	0/1685	0.45	0/2262
35	2d	0.28	0/1704	0.46	0/2284
36	1e	0.30	0/1145	0.51	0/1543
36	2e	0.30	0/1149	0.51	0/1548
37	1f	0.28	0/823	0.49	0/1115
37	2f	0.27	0/829	0.47	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.27	0/1250	0.42	0/1679
38	2g	0.27	0/1254	0.42	0/1683
39	1h	0.28	0/1108	0.49	0/1494
39	2h	0.27	0/1108	0.47	0/1494
40	1i	0.28	0/1002	0.48	0/1346
40	2i	0.29	0/997	0.51	0/1343
41	1j	0.26	0/722	0.48	0/982
41	2j	0.28	0/727	0.55	0/988
42	1k	0.28	0/844	0.50	0/1145
42	2k	0.28	0/848	0.47	0/1149
43	1l	0.28	0/937	0.51	0/1260
43	2l	0.28	0/937	0.49	0/1260
44	1m	0.27	0/969	0.46	0/1302
44	2m	0.28	0/961	0.45	0/1291
45	1n	0.29	0/501	0.45	0/664
45	2n	0.30	0/501	0.49	0/664
46	1o	0.27	0/739	0.44	0/985
46	2o	0.26	0/739	0.41	0/985
47	1p	0.28	0/697	0.51	0/939
47	2p	0.27	0/693	0.51	0/935
48	1q	0.27	0/836	0.48	0/1117
48	2q	0.27	0/836	0.47	0/1117
49	1r	0.28	0/560	0.46	0/746
49	2r	0.26	0/560	0.44	0/746
50	1s	0.26	0/667	0.51	0/900
50	2s	0.31	0/661	0.53	0/893
51	1t	0.28	0/730	0.46	0/965
51	2t	0.26	0/729	0.43	0/965
52	1u	0.27	0/203	0.46	0/266
52	2u	0.31	0/203	0.49	0/266
53	1v	0.46	0/322	0.87	0/501
53	2v	0.42	0/322	0.79	0/501
54	1w	0.51	1/1639 (0.1%)	1.05	2/2548 (0.1%)
54	2w	0.51	1/1616 (0.1%)	1.04	4/2510 (0.2%)
55	1x	0.56	2/1723 (0.1%)	1.09	15/2684 (0.6%)
55	2x	0.50	1/1723 (0.1%)	1.01	9/2684 (0.3%)
56	1z	0.30	0/10	0.66	0/12
56	2z	0.22	0/10	0.41	0/12
57	1y	0.55	1/1664 (0.1%)	1.02	2/2587 (0.1%)
57	2y	0.55	1/1664 (0.1%)	1.14	6/2587 (0.2%)
All	All	0.39	11/316960 (0.0%)	0.81	225/474542 (0.0%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	2F	0	1
11	1P	0	1
11	2P	0	1
21	1Z	0	1
All	All	0	4

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	1x	1	C	OP3-P	-10.47	1.48	1.61
55	2x	1	C	OP3-P	-10.19	1.49	1.61
2	2B	1	U	OP3-P	-10.18	1.49	1.61
57	2y	1	G	OP3-P	-10.18	1.49	1.61
57	1y	1	G	OP3-P	-10.16	1.49	1.61
54	1w	1	G	OP3-P	-10.05	1.49	1.61
2	1B	1	U	OP3-P	-10.04	1.49	1.61
54	2w	1	G	OP3-P	-10.04	1.49	1.61
32	2a	1272	G	N1-C2	-7.50	1.31	1.37
32	2a	1272	G	C6-N1	-6.90	1.34	1.39
55	1x	14	A	N7-C5	-5.59	1.35	1.39

All (225) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1263	C	N1-C2-O2	19.57	130.65	118.90
32	2a	1272	G	N3-C2-N2	18.76	133.03	119.90
32	2a	1272	G	N1-C2-N2	-16.11	101.70	116.20
32	2a	1272	G	C5-C6-O6	14.10	137.06	128.60
32	2a	1263	C	C2-N3-C4	13.11	126.45	119.90
32	2a	1263	C	C5-C6-N1	11.24	126.62	121.00
1	2A	2136	C	N1-C2-O2	10.82	125.39	118.90
1	2A	1639	U	O5'-P-OP2	-10.65	96.11	105.70
1	1A	2036	C	O5'-P-OP1	-10.27	96.46	105.70
55	1x	14	A	C4-C5-C6	10.09	122.04	117.00
32	2a	1272	G	C6-N1-C2	10.05	131.13	125.10
32	2a	1263	C	N3-C2-O2	-9.97	114.92	121.90
55	1x	46	G	C6-N1-C2	-9.82	119.20	125.10
1	1A	1086	A	N1-C6-N6	-9.78	112.73	118.60
1	1A	1075	C	N1-C2-O2	9.20	124.42	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1272	G	C5-C6-N1	-9.14	106.93	111.50
55	1x	14	A	C5-N7-C8	9.12	108.46	103.90
1	1A	975	C	N1-C2-O2	-8.95	113.53	118.90
55	2x	46	G	C6-N1-C2	-8.86	119.79	125.10
1	1A	801	G	O5'-P-OP2	-8.83	97.75	105.70
1	1A	1063	G	C5-C6-O6	8.83	133.90	128.60
1	1A	1075	C	C2-N3-C4	8.47	124.14	119.90
1	1A	512	G	O4'-C1'-N9	8.44	114.95	108.20
1	1A	2682	U	O5'-P-OP2	-8.43	98.11	105.70
1	2A	2136	C	N3-C2-O2	-8.41	116.01	121.90
32	2a	1272	G	C4-N9-C1'	8.27	137.25	126.50
1	1A	2248	C	O5'-P-OP2	-8.11	98.40	105.70
2	2B	80	U	O4'-C1'-N1	8.04	114.63	108.20
32	2a	1272	G	C8-N9-C1'	-8.00	116.60	127.00
55	1x	14	A	C5-C6-N1	-7.92	113.74	117.70
1	1A	787	U	O5'-P-OP1	-7.82	98.66	105.70
32	2a	754	C	C2-N1-C1'	7.74	127.32	118.80
1	1A	1352	U	O5'-P-OP1	-7.74	98.74	105.70
32	2a	1263	C	C2-N1-C1'	7.66	127.23	118.80
32	2a	1263	C	C4-C5-C6	-7.55	113.62	117.40
1	1A	1063	G	C6-N1-C2	7.54	129.62	125.10
1	1A	1776	G	O5'-P-OP2	-7.52	98.93	105.70
55	1x	22	G	C5-N7-C8	-7.43	100.59	104.30
1	1A	392	C	O5'-P-OP1	-7.35	99.08	105.70
57	2y	48	C	P-O3'-C3'	7.35	128.52	119.70
32	2a	1029	C	N1-C2-O2	7.33	123.30	118.90
32	1a	1034	G	C5-C6-O6	7.33	133.00	128.60
32	2a	1263	C	C6-N1-C2	-7.31	117.38	120.30
32	1a	841	U	C2-N1-C1'	7.28	126.43	117.70
55	2x	14	A	C4-C5-C6	7.27	120.64	117.00
55	1x	46	G	N3-C2-N2	-7.26	114.82	119.90
32	1a	841	U	C5-C6-N1	7.18	126.29	122.70
1	1A	570	G	C5-C6-O6	-7.07	124.36	128.60
1	2A	2155	G	N3-C2-N2	7.04	124.83	119.90
1	1A	2167	U	C2-N1-C1'	7.04	126.15	117.70
1	1A	1394	U	O5'-P-OP1	-6.94	99.46	105.70
32	2a	1263	C	N1-C2-N3	-6.84	114.42	119.20
32	1a	1034	G	C6-N1-C2	6.80	129.18	125.10
32	2a	754	C	N1-C2-O2	6.78	122.97	118.90
55	2x	14	A	C5-N7-C8	6.75	107.28	103.90
1	2A	512	G	O4'-C1'-N9	6.74	113.59	108.20
1	2A	2689	U	N3-C2-O2	-6.73	117.49	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1272	G	C2-N3-C4	-6.68	108.56	111.90
1	1A	624	C	O5'-P-OP1	-6.65	99.72	105.70
1	2A	1298	C	O5'-P-OP2	-6.61	99.75	105.70
1	2A	141	A	N7-C8-N9	6.57	117.08	113.80
32	2a	1272	G	N1-C6-O6	-6.51	115.99	119.90
1	1A	1992	G	P-O3'-C3'	6.48	127.47	119.70
1	1A	226	G	O4'-C1'-N9	6.46	113.37	108.20
55	1x	22	G	C5-C6-N1	6.45	114.73	111.50
32	1a	1030	C	N1-C2-O2	6.43	122.76	118.90
1	1A	1696	G	O5'-P-OP2	-6.42	99.92	105.70
22	10	12	ASN	C-N-CA	-6.42	108.82	122.30
32	2a	1225	A	C5-C6-N6	6.41	128.83	123.70
32	1a	266	G	P-O3'-C3'	6.40	127.38	119.70
1	1A	1272	A	O5'-P-OP2	-6.34	99.99	105.70
55	1x	22	G	C4-C5-C6	-6.34	114.99	118.80
54	2w	14	A	C5-C6-N6	-6.32	118.64	123.70
1	1A	746	A	O4'-C1'-N9	6.31	113.25	108.20
32	2a	1225	A	N1-C6-N6	-6.29	114.82	118.60
32	1a	254	G	O5'-P-OP1	-6.29	100.04	105.70
57	2y	69	C	C2-N3-C4	6.25	123.03	119.90
1	1A	819	A	O5'-P-OP1	-6.24	100.08	105.70
1	1A	446	G	C5-C6-O6	-6.24	124.86	128.60
57	2y	48	C	OP2-P-O3'	6.23	118.90	105.20
1	1A	2175	C	C2-N3-C4	6.21	123.00	119.90
55	1x	46	G	C5-C6-N1	6.20	114.60	111.50
1	1A	1176	G	OP1-P-O3'	6.16	118.75	105.20
1	1A	1187	G	N1-C6-O6	-6.15	116.21	119.90
1	1A	2848	G	O4'-C1'-N9	6.14	113.11	108.20
1	2A	1352	U	O5'-P-OP1	-6.09	100.22	105.70
32	2a	754	C	C6-N1-C1'	-6.08	113.50	120.80
1	1A	2554	U	O5'-P-OP1	-6.07	100.24	105.70
1	2A	1992	G	P-O3'-C3'	6.01	126.92	119.70
1	1A	120	U	O5'-P-OP1	-6.00	100.30	105.70
57	2y	69	C	N1-C2-O2	6.00	122.50	118.90
1	2A	2155	G	C6-N1-C2	5.97	128.68	125.10
1	1A	2167	U	N1-C2-O2	5.96	126.97	122.80
1	1A	2685	G	N1-C6-O6	-5.96	116.32	119.90
32	2a	563	A	O4'-C1'-N9	5.96	112.97	108.20
1	1A	2629	A	P-O3'-C3'	5.95	126.84	119.70
32	1a	90	U	N3-C2-O2	-5.93	118.05	122.20
1	1A	531	C	O5'-P-OP2	-5.93	100.36	105.70
2	2B	1	U	C2-N1-C1'	5.88	124.75	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2593	U	N3-C4-O4	-5.86	115.30	119.40
32	1a	754	C	N1-C2-O2	5.86	122.42	118.90
32	1a	1531	A	N7-C8-N9	5.86	116.73	113.80
1	2A	1698	A	O4'-C1'-N9	5.85	112.88	108.20
1	2A	847	U	C2-N1-C1'	5.83	124.69	117.70
55	2x	22	G	C5-N7-C8	-5.82	101.39	104.30
32	1a	1025	U	N1-C2-O2	5.78	126.84	122.80
32	2a	1272	G	N3-C4-N9	5.78	129.47	126.00
1	1A	975	C	C2-N1-C1'	-5.77	112.45	118.80
54	2w	14	A	N1-C6-N6	5.76	122.06	118.60
1	1A	576	U	O5'-P-OP1	-5.74	100.53	105.70
32	2a	955	U	C2-N3-C4	5.74	130.44	127.00
1	1A	1075	C	C5-C4-N4	5.72	124.20	120.20
32	2a	266	G	P-O3'-C3'	5.72	126.56	119.70
1	1A	1131	G	O4'-C1'-N9	5.71	112.77	108.20
1	1A	2790	A	C2-N3-C4	5.71	113.45	110.60
32	2a	841	U	C5-C6-N1	5.70	125.55	122.70
1	2A	141	A	C8-N9-C4	-5.69	103.52	105.80
1	1A	740	U	O5'-P-OP2	-5.68	100.58	105.70
1	2A	1380	G	O5'-P-OP2	-5.68	100.59	105.70
1	1A	1236	G	C8-N9-C4	5.68	108.67	106.40
1	1A	568	U	C5-C4-O4	-5.65	122.51	125.90
1	1A	962	G	OP2-P-O3'	5.64	117.61	105.20
57	1y	58	A	OP1-P-O3'	5.64	117.61	105.20
1	1A	2055	C	OP1-P-O3'	5.63	117.59	105.20
55	1x	22	G	C8-N9-C1'	5.63	134.32	127.00
55	2x	22	G	N1-C6-O6	-5.62	116.53	119.90
1	1A	1313	U	C2-N1-C1'	5.61	124.44	117.70
1	2A	787	U	O5'-P-OP1	-5.61	100.65	105.70
1	1A	975	C	C6-N1-C1'	5.59	127.50	120.80
1	1A	847	U	C2-N1-C1'	5.58	124.40	117.70
1	1A	845	G	O4'-C1'-N9	5.58	112.66	108.20
1	2A	1313	U	C2-N1-C1'	5.56	124.38	117.70
32	2a	1158	C	N1-C2-O2	5.54	122.22	118.90
1	1A	333	G	C4-N9-C1'	5.54	133.70	126.50
1	1A	944	G	C8-N9-C1'	-5.51	119.84	127.00
1	1A	784	A	O4'-C1'-N9	5.50	112.60	108.20
32	1a	1158	C	N1-C2-O2	5.49	122.19	118.90
32	2a	1158	C	C2-N1-C1'	5.49	124.83	118.80
32	1a	1030(B)	C	C2-N1-C1'	5.47	124.81	118.80
1	1A	446	G	N1-C6-O6	5.43	123.16	119.90
1	1A	1063	G	N3-C2-N2	5.43	123.70	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	944	G	N3-C4-N9	5.43	129.26	126.00
1	1A	2789	C	C2-N1-C1'	-5.42	112.84	118.80
1	2A	2689	U	P-O3'-C3'	5.41	126.19	119.70
55	2x	22	G	C5-C6-N1	5.41	114.20	111.50
1	1A	450	G	N1-C6-O6	-5.40	116.66	119.90
32	2a	1029	C	N3-C2-O2	-5.39	118.13	121.90
1	1A	1969	A	OP1-P-O3'	5.38	117.04	105.20
1	1A	1075	C	N3-C2-O2	-5.38	118.13	121.90
1	2A	2804	C	C6-N1-C2	-5.37	118.15	120.30
32	1a	267	C	O5'-P-OP1	-5.35	100.88	105.70
1	1A	1174	A	P-O3'-C3'	5.35	126.12	119.70
1	2A	1204	A	O4'-C1'-N9	5.34	112.47	108.20
1	2A	228	A	P-O3'-C3'	5.34	126.11	119.70
1	1A	944	G	C6-C5-N7	-5.34	127.20	130.40
54	2w	25	C	C2-N1-C1'	5.33	124.66	118.80
1	2A	271(M)	G	P-O3'-C3'	5.33	126.09	119.70
1	1A	793	A	O5'-P-OP2	-5.32	100.91	105.70
1	1A	195	A	P-O3'-C3'	5.31	126.07	119.70
1	2A	741	G	O5'-P-OP1	-5.30	100.93	105.70
1	2A	277	C	OP2-P-O3'	5.29	116.83	105.20
1	1A	944	G	C4-N9-C1'	5.27	133.35	126.50
32	1a	90	U	N1-C2-O2	5.26	126.48	122.80
1	2A	2447	G	C4-N9-C1'	-5.26	119.66	126.50
32	1a	1158	C	C2-N1-C1'	5.25	124.58	118.80
1	1A	1380	G	O5'-P-OP2	-5.25	100.98	105.70
1	1A	1936	A	O4'-C1'-N9	5.25	112.40	108.20
55	1x	14	A	C4-N9-C1'	5.24	135.74	126.30
55	2x	46	G	C5-C6-N1	5.24	114.12	111.50
1	2A	2689	U	N1-C2-O2	5.24	126.47	122.80
57	2y	70	C	N1-C2-O2	5.24	122.04	118.90
1	1A	1647	G	O4'-C1'-N9	-5.22	104.02	108.20
1	1A	570	G	N3-C4-N9	5.22	129.13	126.00
1	2A	1420	U	P-O3'-C3'	5.21	125.95	119.70
1	2A	2430	A	O4'-C1'-N9	5.21	112.36	108.20
54	2w	25	C	C6-N1-C2	-5.19	118.22	120.30
1	2A	528	A	OP1-P-O3'	5.18	116.61	105.20
1	1A	2553	G	N3-C4-N9	5.18	129.11	126.00
32	2a	687	A	P-O3'-C3'	5.18	125.91	119.70
1	2A	271(M)	G	OP1-P-O3'	5.17	116.58	105.20
54	1w	44	A	C5-C6-N6	5.17	127.84	123.70
1	1A	1174	A	OP1-P-O3'	5.17	116.57	105.20
1	1A	570	G	C5-C6-N1	5.17	114.08	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1082	U	N3-C4-O4	-5.17	115.78	119.40
1	1A	2492	U	O5'-P-OP1	-5.17	101.05	105.70
1	2A	141	A	O4'-C1'-N9	5.16	112.33	108.20
55	1x	46	G	C5-C6-O6	-5.16	125.50	128.60
55	1x	14	A	C8-N9-C1'	-5.16	118.42	127.70
55	2x	22	G	C4-C5-C6	-5.16	115.71	118.80
57	1y	58	A	P-O3'-C3'	5.15	125.88	119.70
32	2a	1054	C	C2-N1-C1'	5.15	124.46	118.80
1	1A	570	G	C4-C5-N7	5.15	112.86	110.80
1	1A	1992	G	O4'-C1'-N9	-5.14	104.09	108.20
1	1A	12	U	N3-C2-O2	-5.13	118.61	122.20
1	1A	1190	G	C5-N7-C8	5.13	106.86	104.30
1	1A	2598	A	O5'-P-OP1	-5.11	101.10	105.70
1	2A	2155	G	N9-C4-C5	-5.11	103.36	105.40
32	1a	841	U	N1-C2-O2	5.11	126.38	122.80
32	1a	754	C	C2-N1-C1'	5.11	124.42	118.80
1	1A	1542	A	O5'-P-OP1	-5.10	101.11	105.70
55	2x	14	A	C5-C6-N1	-5.10	115.15	117.70
16	2U	74	LEU	CA-CB-CG	5.10	127.03	115.30
55	1x	46	G	N9-C4-C5	5.09	107.44	105.40
32	1a	913	A	P-O3'-C3'	5.09	125.80	119.70
1	1A	450	G	C5-C6-N1	5.08	114.04	111.50
1	1A	1385	G	O4'-C1'-N9	5.07	112.26	108.20
1	1A	372	G	O4'-C1'-N9	5.06	112.25	108.20
55	1x	14	A	C4-C5-N7	-5.05	108.17	110.70
32	2a	913	A	P-O3'-C3'	5.05	125.76	119.70
1	1A	2206	G	C4-N9-C1'	-5.04	119.94	126.50
1	2A	528	A	P-O3'-C3'	5.04	125.75	119.70
1	2A	1791	A	O5'-P-OP1	-5.04	101.16	105.70
32	2a	65	U	P-O3'-C3'	5.04	125.75	119.70
32	2a	1264	C	N1-C2-O2	5.04	121.92	118.90
57	2y	33	U	N3-C2-O2	-5.04	118.67	122.20
1	1A	975	C	N1-C2-N3	5.03	122.72	119.20
32	1a	841	U	C6-N1-C2	-5.03	117.98	121.00
1	1A	2059	A	O4'-C1'-N9	5.02	112.22	108.20
1	1A	1082	U	N3-C4-C5	5.02	117.61	114.60
32	1a	1067	A	P-O3'-C3'	5.02	125.72	119.70
1	1A	383	U	C2-N1-C1'	-5.02	111.68	117.70
32	1a	115	G	P-O3'-C3'	5.01	125.72	119.70
54	1w	44	A	N1-C6-N6	-5.01	115.59	118.60
1	1A	2167	U	N3-C2-O2	-5.01	118.69	122.20
32	2a	754	C	N3-C2-O2	-5.00	118.40	121.90

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	1P	35	HIS	Peptide
21	1Z	136	PHE	Peptide
5	2F	20	LEU	Peptide
11	2P	35	HIS	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%)	259 (95%)	14 (5%)	0	100	100
3	2D	273/276 (99%)	257 (94%)	16 (6%)	0	100	100
4	1E	202/206 (98%)	194 (96%)	7 (4%)	1 (0%)	29	40
4	2E	202/206 (98%)	191 (95%)	10 (5%)	1 (0%)	29	40
5	1F	200/210 (95%)	195 (98%)	4 (2%)	1 (0%)	29	40
5	2F	200/210 (95%)	191 (96%)	7 (4%)	2 (1%)	15	22
6	1G	179/182 (98%)	165 (92%)	13 (7%)	1 (1%)	25	34
6	2G	179/182 (98%)	160 (89%)	17 (10%)	2 (1%)	14	19
7	1H	172/180 (96%)	161 (94%)	10 (6%)	1 (1%)	25	34
7	2H	172/180 (96%)	158 (92%)	11 (6%)	3 (2%)	9	11
8	1I	144/148 (97%)	130 (90%)	14 (10%)	0	100	100
8	2I	144/148 (97%)	125 (87%)	17 (12%)	2 (1%)	11	15
9	1N	138/140 (99%)	133 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	2N	138/140 (99%)	131 (95%)	5 (4%)	2 (1%)	11	15
10	1O	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
10	2O	120/122 (98%)	112 (93%)	7 (6%)	1 (1%)	19	27
11	1P	147/150 (98%)	135 (92%)	10 (7%)	2 (1%)	11	15
11	2P	147/150 (98%)	130 (88%)	16 (11%)	1 (1%)	22	30
12	1Q	139/141 (99%)	129 (93%)	10 (7%)	0	100	100
12	2Q	139/141 (99%)	128 (92%)	10 (7%)	1 (1%)	22	30
13	1R	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
13	2R	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
14	1S	108/112 (96%)	99 (92%)	9 (8%)	0	100	100
14	2S	108/112 (96%)	97 (90%)	8 (7%)	3 (3%)	5	4
15	1T	129/146 (88%)	121 (94%)	8 (6%)	0	100	100
15	2T	129/146 (88%)	119 (92%)	9 (7%)	1 (1%)	19	27
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%)	95 (96%)	4 (4%)	0	100	100
17	2V	99/101 (98%)	91 (92%)	7 (7%)	1 (1%)	15	22
18	1W	110/113 (97%)	110 (100%)	0	0	100	100
18	2W	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
19	1X	93/96 (97%)	88 (95%)	4 (4%)	1 (1%)	14	19
19	2X	93/96 (97%)	87 (94%)	6 (6%)	0	100	100
20	1Y	105/110 (96%)	98 (93%)	6 (6%)	1 (1%)	15	22
20	2Y	105/110 (96%)	100 (95%)	5 (5%)	0	100	100
21	1Z	148/206 (72%)	134 (90%)	13 (9%)	1 (1%)	22	30
21	2Z	156/206 (76%)	130 (83%)	25 (16%)	1 (1%)	25	34
22	10	81/85 (95%)	80 (99%)	1 (1%)	0	100	100
22	20	81/85 (95%)	76 (94%)	5 (6%)	0	100	100
23	11	95/98 (97%)	94 (99%)	0	1 (1%)	14	19
23	21	95/98 (97%)	92 (97%)	3 (3%)	0	100	100
24	12	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
24	22	68/72 (94%)	66 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	13	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
25	23	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
26	14	67/71 (94%)	54 (81%)	9 (13%)	4 (6%)	1	0
26	24	67/71 (94%)	53 (79%)	9 (13%)	5 (8%)	1	0
27	15	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	25	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
28	16	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
28	26	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
29	17	46/49 (94%)	46 (100%)	0	0	100	100
29	27	46/49 (94%)	46 (100%)	0	0	100	100
30	18	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
30	28	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
33	1b	229/256 (90%)	189 (82%)	34 (15%)	6 (3%)	5	5
33	2b	229/256 (90%)	180 (79%)	41 (18%)	8 (4%)	3	2
34	1c	204/239 (85%)	184 (90%)	19 (9%)	1 (0%)	29	40
34	2c	204/239 (85%)	173 (85%)	27 (13%)	4 (2%)	7	8
35	1d	206/209 (99%)	189 (92%)	15 (7%)	2 (1%)	15	22
35	2d	206/209 (99%)	192 (93%)	13 (6%)	1 (0%)	29	40
36	1e	146/162 (90%)	128 (88%)	15 (10%)	3 (2%)	7	7
36	2e	146/162 (90%)	129 (88%)	13 (9%)	4 (3%)	5	4
37	1f	98/101 (97%)	92 (94%)	6 (6%)	0	100	100
37	2f	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
38	1g	153/156 (98%)	141 (92%)	12 (8%)	0	100	100
38	2g	153/156 (98%)	137 (90%)	13 (8%)	3 (2%)	7	8
39	1h	135/138 (98%)	126 (93%)	9 (7%)	0	100	100
39	2h	135/138 (98%)	125 (93%)	10 (7%)	0	100	100
40	1i	125/128 (98%)	105 (84%)	18 (14%)	2 (2%)	9	12
40	2i	125/128 (98%)	105 (84%)	20 (16%)	0	100	100
41	1j	95/105 (90%)	84 (88%)	8 (8%)	3 (3%)	4	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	2j	94/105 (90%)	80 (85%)	12 (13%)	2 (2%)	7	7
42	1k	112/129 (87%)	103 (92%)	7 (6%)	2 (2%)	8	10
42	2k	112/129 (87%)	105 (94%)	5 (4%)	2 (2%)	8	10
43	1l	119/132 (90%)	110 (92%)	8 (7%)	1 (1%)	19	27
43	2l	119/132 (90%)	109 (92%)	9 (8%)	1 (1%)	19	27
44	1m	121/126 (96%)	109 (90%)	11 (9%)	1 (1%)	19	27
44	2m	120/126 (95%)	105 (88%)	12 (10%)	3 (2%)	5	5
45	1n	58/61 (95%)	53 (91%)	5 (9%)	0	100	100
45	2n	58/61 (95%)	54 (93%)	4 (7%)	0	100	100
46	1o	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
46	2o	86/89 (97%)	80 (93%)	6 (7%)	0	100	100
47	1p	80/88 (91%)	65 (81%)	15 (19%)	0	100	100
47	2p	80/88 (91%)	72 (90%)	7 (9%)	1 (1%)	12	16
48	1q	97/105 (92%)	92 (95%)	5 (5%)	0	100	100
48	2q	97/105 (92%)	91 (94%)	5 (5%)	1 (1%)	15	22
49	1r	66/88 (75%)	56 (85%)	10 (15%)	0	100	100
49	2r	66/88 (75%)	62 (94%)	3 (4%)	1 (2%)	10	14
50	1s	81/93 (87%)	72 (89%)	9 (11%)	0	100	100
50	2s	81/93 (87%)	66 (82%)	12 (15%)	3 (4%)	3	2
51	1t	94/106 (89%)	85 (90%)	6 (6%)	3 (3%)	4	3
51	2t	94/106 (89%)	86 (92%)	6 (6%)	2 (2%)	7	7
52	1u	21/27 (78%)	18 (86%)	3 (14%)	0	100	100
52	2u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
56	1z	1/3 (33%)	0	1 (100%)	0	100	100
56	2z	1/3 (33%)	1 (100%)	0	0	100	100
All	All	11370/12134 (94%)	10453 (92%)	817 (7%)	100 (1%)	17	24

All (100) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
26	14	47	GLN
26	14	62	ARG

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Mol	Chain	Res	Type
33	1b	17	PHE
33	1b	22	LYS
35	1d	173	TRP
42	1k	49	GLY
44	1m	67	GLU
5	2F	130	ALA
6	2G	51	ARG
33	2b	17	PHE
33	2b	121	LEU
38	2g	55	GLY
38	2g	80	VAL
6	1G	43	LEU
19	1X	93	GLU
21	1Z	52	SER
23	1l	3	LYS
33	1b	227	GLY
36	1e	85	GLY
40	1i	54	ASP
51	1t	47	GLY
6	2G	47	LYS
7	2H	47	GLU
10	2O	5	GLN
26	24	45	GLY
26	24	54	GLY
33	2b	21	ARG
33	2b	123	ALA
34	2c	156	ARG
34	2c	181	ASN
36	2e	65	ASN
36	2e	85	GLY
42	2k	49	GLY
44	2m	5	ALA
44	2m	67	GLU
51	2t	47	GLY
7	1H	159	GLU
26	14	49	PHE
35	1d	172	PRO
42	1k	77	MET
4	2E	52	LEU
7	2H	126	PRO
14	2S	20	ARG
21	2Z	52	SER

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Mol	Chain	Res	Type
33	2b	9	GLU
33	2b	20	GLU
50	2s	81	ARG
4	1E	52	LEU
11	1P	45	LEU
33	1b	20	GLU
33	1b	231	GLU
41	1j	78	ASN
43	1l	105	TYR
8	2I	49	ALA
9	2N	2	LYS
9	2N	23	LEU
14	2S	84	GLN
14	2S	96	GLY
26	24	50	VAL
34	2c	91	LEU
34	2c	95	THR
35	2d	179	GLU
41	2j	79	ARG
43	2l	105	TYR
44	2m	58	GLU
48	2q	68	ARG
50	2s	13	ASP
50	2s	70	LYS
51	2t	95	ALA
20	1Y	54	LYS
26	14	53	GLU
33	1b	125	PRO
36	1e	69	VAL
41	1j	29	ARG
41	1j	77	PRO
8	2I	10	GLU
11	2P	45	LEU
26	24	49	PHE
33	2b	120	ALA
33	2b	125	PRO
38	2g	4	ARG
41	2j	78	ASN
49	2r	25	THR
36	1e	86	ALA
51	1t	102	GLY
12	2Q	60	ARG

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Mol	Chain	Res	Type
15	2T	127	ALA
26	24	65	ASP
36	2e	37	ARG
36	2e	77	PRO
5	2F	206	ILE
34	1c	81	GLY
40	1i	53	VAL
11	1P	122	PRO
7	2H	21	PRO
42	2k	105	VAL
47	2p	78	GLY
51	1t	100	ILE
17	2V	50	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	215/218 (99%)	206 (96%)	9 (4%)	30	40
3	2D	215/218 (99%)	207 (96%)	8 (4%)	34	46
4	1E	164/166 (99%)	155 (94%)	9 (6%)	21	29
4	2E	164/166 (99%)	158 (96%)	6 (4%)	34	46
5	1F	160/166 (96%)	148 (92%)	12 (8%)	13	17
5	2F	159/166 (96%)	152 (96%)	7 (4%)	28	38
6	1G	143/156 (92%)	131 (92%)	12 (8%)	11	13
6	2G	143/156 (92%)	120 (84%)	23 (16%)	2	2
7	1H	144/148 (97%)	136 (94%)	8 (6%)	21	28
7	2H	144/148 (97%)	130 (90%)	14 (10%)	8	9
8	1I	113/124 (91%)	102 (90%)	11 (10%)	8	9
8	2I	105/124 (85%)	89 (85%)	16 (15%)	3	2
9	1N	118/119 (99%)	112 (95%)	6 (5%)	24	32
9	2N	118/119 (99%)	110 (93%)	8 (7%)	16	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	1O	100/100 (100%)	97 (97%)	3 (3%)	41	55
10	2O	100/100 (100%)	98 (98%)	2 (2%)	55	70
11	1P	115/116 (99%)	111 (96%)	4 (4%)	36	49
11	2P	115/116 (99%)	112 (97%)	3 (3%)	46	61
12	1Q	111/111 (100%)	106 (96%)	5 (4%)	27	37
12	2Q	111/111 (100%)	104 (94%)	7 (6%)	18	23
13	1R	101/101 (100%)	98 (97%)	3 (3%)	41	55
13	2R	101/101 (100%)	100 (99%)	1 (1%)	76	84
14	1S	86/88 (98%)	82 (95%)	4 (5%)	26	35
14	2S	85/88 (97%)	79 (93%)	6 (7%)	14	19
15	1T	115/127 (91%)	109 (95%)	6 (5%)	23	30
15	2T	113/127 (89%)	109 (96%)	4 (4%)	36	49
16	1U	93/94 (99%)	90 (97%)	3 (3%)	39	53
16	2U	93/94 (99%)	88 (95%)	5 (5%)	22	29
17	1V	80/82 (98%)	78 (98%)	2 (2%)	47	62
17	2V	80/82 (98%)	74 (92%)	6 (8%)	13	17
18	1W	90/92 (98%)	84 (93%)	6 (7%)	16	21
18	2W	90/92 (98%)	87 (97%)	3 (3%)	38	51
19	1X	77/78 (99%)	77 (100%)	0	100	100
19	2X	77/78 (99%)	76 (99%)	1 (1%)	69	80
20	1Y	85/91 (93%)	76 (89%)	9 (11%)	6	7
20	2Y	85/91 (93%)	78 (92%)	7 (8%)	11	14
21	1Z	135/179 (75%)	123 (91%)	12 (9%)	9	12
21	2Z	137/179 (76%)	124 (90%)	13 (10%)	8	10
22	10	65/67 (97%)	65 (100%)	0	100	100
22	20	65/67 (97%)	62 (95%)	3 (5%)	27	36
23	11	80/83 (96%)	77 (96%)	3 (4%)	33	45
23	21	80/83 (96%)	77 (96%)	3 (4%)	33	45
24	12	65/67 (97%)	61 (94%)	4 (6%)	18	24
24	22	65/67 (97%)	62 (95%)	3 (5%)	27	36
25	13	51/52 (98%)	49 (96%)	2 (4%)	32	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	23	50/52 (96%)	47 (94%)	3 (6%)	19	25
26	14	59/63 (94%)	53 (90%)	6 (10%)	7	8
26	24	53/63 (84%)	47 (89%)	6 (11%)	6	5
27	15	50/52 (96%)	46 (92%)	4 (8%)	12	15
27	25	50/52 (96%)	47 (94%)	3 (6%)	19	25
28	16	51/52 (98%)	48 (94%)	3 (6%)	19	25
28	26	50/52 (96%)	43 (86%)	7 (14%)	3	3
29	17	41/42 (98%)	37 (90%)	4 (10%)	8	9
29	27	41/42 (98%)	38 (93%)	3 (7%)	14	18
30	18	54/55 (98%)	49 (91%)	5 (9%)	9	10
30	28	54/55 (98%)	49 (91%)	5 (9%)	9	10
31	19	34/34 (100%)	34 (100%)	0	100	100
31	29	34/34 (100%)	33 (97%)	1 (3%)	42	57
33	1b	192/220 (87%)	176 (92%)	16 (8%)	11	14
33	2b	187/220 (85%)	164 (88%)	23 (12%)	4	4
34	1c	142/188 (76%)	124 (87%)	18 (13%)	4	4
34	2c	140/188 (74%)	127 (91%)	13 (9%)	9	10
35	1d	169/181 (93%)	155 (92%)	14 (8%)	11	14
35	2d	173/181 (96%)	159 (92%)	14 (8%)	11	14
36	1e	113/123 (92%)	107 (95%)	6 (5%)	22	30
36	2e	114/123 (93%)	99 (87%)	15 (13%)	4	3
37	1f	84/90 (93%)	79 (94%)	5 (6%)	19	25
37	2f	85/90 (94%)	79 (93%)	6 (7%)	14	19
38	1g	119/127 (94%)	108 (91%)	11 (9%)	9	11
38	2g	120/127 (94%)	110 (92%)	10 (8%)	11	14
39	1h	114/119 (96%)	107 (94%)	7 (6%)	18	24
39	2h	114/119 (96%)	104 (91%)	10 (9%)	10	12
40	1i	90/99 (91%)	78 (87%)	12 (13%)	4	3
40	2i	89/99 (90%)	77 (86%)	12 (14%)	4	3
41	1j	66/92 (72%)	56 (85%)	10 (15%)	3	2
41	2j	69/92 (75%)	60 (87%)	9 (13%)	4	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	1k	82/99 (83%)	78 (95%)	4 (5%)	25	34
42	2k	83/99 (84%)	74 (89%)	9 (11%)	6	6
43	1l	96/108 (89%)	91 (95%)	5 (5%)	23	30
43	2l	96/108 (89%)	88 (92%)	8 (8%)	11	14
44	1m	93/101 (92%)	86 (92%)	7 (8%)	13	17
44	2m	92/101 (91%)	83 (90%)	9 (10%)	8	9
45	1n	49/50 (98%)	43 (88%)	6 (12%)	5	4
45	2n	49/50 (98%)	43 (88%)	6 (12%)	5	4
46	1o	78/80 (98%)	75 (96%)	3 (4%)	33	45
46	2o	78/80 (98%)	76 (97%)	2 (3%)	46	61
47	1p	69/74 (93%)	60 (87%)	9 (13%)	4	3
47	2p	68/74 (92%)	62 (91%)	6 (9%)	10	12
48	1q	94/97 (97%)	86 (92%)	8 (8%)	10	13
48	2q	94/97 (97%)	90 (96%)	4 (4%)	29	39
49	1r	59/77 (77%)	54 (92%)	5 (8%)	10	13
49	2r	59/77 (77%)	55 (93%)	4 (7%)	16	20
50	1s	69/80 (86%)	66 (96%)	3 (4%)	29	39
50	2s	67/80 (84%)	61 (91%)	6 (9%)	9	11
51	1t	70/82 (85%)	68 (97%)	2 (3%)	42	57
51	2t	70/82 (85%)	66 (94%)	4 (6%)	20	27
52	1u	18/22 (82%)	18 (100%)	0	100	100
52	2u	18/22 (82%)	18 (100%)	0	100	100
56	1z	1/1 (100%)	1 (100%)	0	100	100
56	2z	1/1 (100%)	1 (100%)	0	100	100
All	All	9305/10066 (92%)	8652 (93%)	653 (7%)	15	19

All (653) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	3	VAL
3	1D	37	LEU
3	1D	122	ASP
3	1D	126	GLN
3	1D	181	GLU

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Mol	Chain	Res	Type
3	1D	211	ARG
3	1D	229	VAL
3	1D	242	ARG
3	1D	259	THR
4	1E	21	VAL
4	1E	59	VAL
4	1E	73	GLU
4	1E	89	ASP
4	1E	93	VAL
4	1E	113	PHE
4	1E	116	VAL
4	1E	181	LEU
4	1E	184	VAL
5	1F	9	ILE
5	1F	24	LEU
5	1F	53	THR
5	1F	57	VAL
5	1F	70	THR
5	1F	74	ARG
5	1F	106	ARG
5	1F	168	ARG
5	1F	175	THR
5	1F	183	VAL
5	1F	192	LEU
5	1F	201	VAL
6	1G	7	LEU
6	1G	31	VAL
6	1G	33	ARG
6	1G	43	LEU
6	1G	64	THR
6	1G	70	VAL
6	1G	79	ASN
6	1G	126	ASP
6	1G	139	LEU
6	1G	148	MET
6	1G	150	ASP
6	1G	159	VAL
7	1H	3	ARG
7	1H	13	LYS
7	1H	15	VAL
7	1H	88	LEU
7	1H	119	GLU

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Mol	Chain	Res	Type
7	1H	122	THR
7	1H	124	GLU
7	1H	134	SER
8	1I	20	ASP
8	1I	38	LEU
8	1I	41	GLU
8	1I	47	LEU
8	1I	57	ARG
8	1I	61	ARG
8	1I	75	LEU
8	1I	78	THR
8	1I	85	GLU
8	1I	86	THR
8	1I	87	LYS
9	1N	1	MET
9	1N	22	THR
9	1N	28	THR
9	1N	71	ILE
9	1N	83	LYS
9	1N	89	LYS
10	1O	20	MET
10	1O	28	SER
10	1O	113	LYS
11	1P	2	LYS
11	1P	3	LEU
11	1P	77	ARG
11	1P	133	SER
12	1Q	1	MET
12	1Q	6	ARG
12	1Q	7	MET
12	1Q	56	ARG
12	1Q	75	THR
13	1R	6	SER
13	1R	67	LEU
13	1R	114	VAL
14	1S	14	VAL
14	1S	36	TYR
14	1S	46	VAL
14	1S	69	VAL
15	1T	28	VAL
15	1T	51	ARG
15	1T	74	ARG

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Mol	Chain	Res	Type
15	1T	96	ARG
15	1T	118	ARG
15	1T	128	GLU
16	1U	5	LYS
16	1U	74	LEU
16	1U	108	GLU
17	1V	28	GLU
17	1V	56	SER
18	1W	4	LYS
18	1W	11	ARG
18	1W	60	ASN
18	1W	63	ASP
18	1W	67	ASP
18	1W	92	ARG
20	1Y	1	MET
20	1Y	7	VAL
20	1Y	8	LYS
20	1Y	43	ASN
20	1Y	50	ARG
20	1Y	55	TYR
20	1Y	67	LEU
20	1Y	91	GLU
20	1Y	99	CYS
21	1Z	18	LEU
21	1Z	46	LYS
21	1Z	49	ARG
21	1Z	61	LEU
21	1Z	66	SER
21	1Z	72	ARG
21	1Z	87	ASP
21	1Z	132	ASN
21	1Z	136	PHE
21	1Z	138	GLU
21	1Z	140	ASP
21	1Z	170	THR
23	11	40	ARG
23	11	57	GLU
23	11	83	GLU
24	12	28	LYS
24	12	40	SER
24	12	50	ILE
24	12	69	ARG

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Mol	Chain	Res	Type
25	13	23	LEU
25	13	60	GLU
26	14	49	PHE
26	14	53	GLU
26	14	59	PHE
26	14	61	ARG
26	14	63	TYR
26	14	67	TYR
27	15	6	VAL
27	15	40	LYS
27	15	57	VAL
27	15	58	LEU
28	16	13	CYS
28	16	14	THR
28	16	19	ARG
29	17	14	LYS
29	17	24	THR
29	17	43	THR
29	17	48	LYS
30	18	14	VAL
30	18	15	LYS
30	18	29	LYS
30	18	31	HIS
30	18	34	TRP
33	1b	7	VAL
33	1b	11	LEU
33	1b	21	ARG
33	1b	24	TRP
33	1b	35	GLU
33	1b	45	GLN
33	1b	48	MET
33	1b	53	ARG
33	1b	67	THR
33	1b	78	GLN
33	1b	107	THR
33	1b	126	GLU
33	1b	138	LEU
33	1b	215	LEU
33	1b	219	VAL
33	1b	230	VAL
34	1c	3	ASN
34	1c	8	ILE

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Mol	Chain	Res	Type
34	1c	16	ARG
34	1c	17	ASP
34	1c	20	SER
34	1c	26	LYS
34	1c	28	GLN
34	1c	29	TYR
34	1c	33	LEU
34	1c	66	VAL
34	1c	89	GLU
34	1c	101	LEU
34	1c	103	VAL
34	1c	119	ARG
34	1c	126	ARG
34	1c	165	THR
34	1c	190	ARG
34	1c	195	VAL
35	1d	3	ARG
35	1d	19	LEU
35	1d	30	LYS
35	1d	31	CYS
35	1d	127	THR
35	1d	135	LEU
35	1d	140	VAL
35	1d	146	ILE
35	1d	158	ILE
35	1d	175	SER
35	1d	177	ASP
35	1d	181	MET
35	1d	190	ASP
35	1d	200	GLU
36	1e	16	THR
36	1e	31	LEU
36	1e	41	VAL
36	1e	78	HIS
36	1e	79	GLU
36	1e	135	THR
37	1f	43	LEU
37	1f	54	LYS
37	1f	55	ASP
37	1f	64	GLN
37	1f	72	VAL
38	1g	12	LEU

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Mol	Chain	Res	Type
38	1g	24	THR
38	1g	32	ARG
38	1g	50	ILE
38	1g	56	GLN
38	1g	89	MET
38	1g	104	LEU
38	1g	106	GLN
38	1g	113	GLU
38	1g	139	GLU
38	1g	156	TRP
39	1h	24	THR
39	1h	26	VAL
39	1h	52	ASP
39	1h	60	ARG
39	1h	109	ILE
39	1h	112	LEU
39	1h	127	LEU
40	1i	17	VAL
40	1i	23	ASN
40	1i	51	ARG
40	1i	53	VAL
40	1i	60	ASP
40	1i	75	ASP
40	1i	83	ARG
40	1i	92	TYR
40	1i	103	THR
40	1i	105	ASP
40	1i	121	ARG
40	1i	128	ARG
41	1j	9	ARG
41	1j	34	VAL
41	1j	43	ARG
41	1j	44	VAL
41	1j	81	THR
41	1j	84	GLN
41	1j	92	THR
41	1j	94	VAL
41	1j	97	GLU
41	1j	98	ILE
42	1k	48	ILE
42	1k	87	THR
42	1k	114	VAL

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Mol	Chain	Res	Type
42	1k	120	ARG
43	1l	18	VAL
43	1l	33	ARG
43	1l	36	VAL
43	1l	40	VAL
43	1l	118	SER
44	1m	4	ILE
44	1m	43	THR
44	1m	64	TRP
44	1m	70	LEU
44	1m	98	VAL
44	1m	108	ARG
44	1m	109	THR
45	1n	3	ARG
45	1n	11	LYS
45	1n	18	VAL
45	1n	33	VAL
45	1n	41	ARG
45	1n	56	VAL
46	1o	5	LYS
46	1o	6	GLU
46	1o	76	GLU
47	1p	1	MET
47	1p	5	ARG
47	1p	19	ILE
47	1p	20	VAL
47	1p	27	LYS
47	1p	49	LEU
47	1p	62	VAL
47	1p	67	THR
47	1p	73	LEU
48	1q	7	THR
48	1q	14	LYS
48	1q	34	LYS
48	1q	53	LEU
48	1q	60	ILE
48	1q	79	SER
48	1q	93	GLN
48	1q	99	SER
49	1r	42	ARG
49	1r	47	THR
49	1r	51	LEU

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Mol	Chain	Res	Type
49	1r	63	GLN
49	1r	65	ILE
50	1s	12	ASP
50	1s	39	THR
50	1s	66	MET
51	1t	10	LEU
51	1t	62	LEU
3	2D	37	LEU
3	2D	38	LYS
3	2D	88	ARG
3	2D	99	ASP
3	2D	211	ARG
3	2D	229	VAL
3	2D	242	ARG
3	2D	259	THR
4	2E	21	VAL
4	2E	73	GLU
4	2E	77	ILE
4	2E	113	PHE
4	2E	116	VAL
4	2E	181	LEU
5	2F	33	LEU
5	2F	60	SER
5	2F	70	THR
5	2F	154	VAL
5	2F	160	ASN
5	2F	165	ARG
5	2F	170	LEU
6	2G	5	VAL
6	2G	7	LEU
6	2G	18	GLU
6	2G	28	VAL
6	2G	31	VAL
6	2G	39	ILE
6	2G	45	GLU
6	2G	49	ASP
6	2G	91	ARG
6	2G	111	LEU
6	2G	116	ASP
6	2G	124	SER
6	2G	126	ASP
6	2G	133	LEU

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Mol	Chain	Res	Type
6	2G	135	LEU
6	2G	137	GLU
6	2G	140	ILE
6	2G	148	MET
6	2G	152	LEU
6	2G	157	ILE
6	2G	165	THR
6	2G	170	ARG
6	2G	173	LEU
7	2H	7	LEU
7	2H	15	VAL
7	2H	24	VAL
7	2H	40	GLU
7	2H	45	VAL
7	2H	47	GLU
7	2H	63	SER
7	2H	68	THR
7	2H	88	LEU
7	2H	104	GLU
7	2H	106	THR
7	2H	119	GLU
7	2H	149	ARG
7	2H	152	ARG
8	2I	7	GLU
8	2I	15	VAL
8	2I	20	ASP
8	2I	38	LEU
8	2I	61	ARG
8	2I	69	LYS
8	2I	79	ILE
8	2I	85	GLU
8	2I	86	THR
8	2I	87	LYS
8	2I	101	LEU
8	2I	108	THR
8	2I	117	GLU
8	2I	129	THR
8	2I	142	VAL
8	2I	144	VAL
9	2N	1	MET
9	2N	22	THR
9	2N	28	THR

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Mol	Chain	Res	Type
9	2N	32	THR
9	2N	43	THR
9	2N	46	VAL
9	2N	48	MET
9	2N	83	LYS
10	2O	28	SER
10	2O	52	VAL
11	2P	29	LYS
11	2P	77	ARG
11	2P	105	LEU
12	2Q	6	ARG
12	2Q	54	MET
12	2Q	56	ARG
12	2Q	75	THR
12	2Q	85	LYS
12	2Q	109	VAL
12	2Q	110	THR
13	2R	67	LEU
14	2S	25	ARG
14	2S	53	SER
14	2S	63	THR
14	2S	75	GLU
14	2S	78	LEU
14	2S	83	LYS
15	2T	64	ARG
15	2T	74	ARG
15	2T	107	ASP
15	2T	125	ARG
16	2U	5	LYS
16	2U	60	LEU
16	2U	74	LEU
16	2U	77	SER
16	2U	108	GLU
17	2V	7	THR
17	2V	15	GLU
17	2V	38	LEU
17	2V	52	VAL
17	2V	73	SER
17	2V	98	GLU
18	2W	11	ARG
18	2W	63	ASP
18	2W	92	ARG

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Mol	Chain	Res	Type
19	2X	38	GLU
20	2Y	6	HIS
20	2Y	9	LYS
20	2Y	28	LYS
20	2Y	45	VAL
20	2Y	91	GLU
20	2Y	99	CYS
20	2Y	101	LYS
21	2Z	5	LEU
21	2Z	33	LEU
21	2Z	35	ARG
21	2Z	42	VAL
21	2Z	72	ARG
21	2Z	98	MET
21	2Z	121	HIS
21	2Z	122	ARG
21	2Z	123	ASP
21	2Z	154	ASP
21	2Z	161	VAL
21	2Z	171	ILE
21	2Z	174	VAL
22	20	10	THR
22	20	11	ARG
22	20	74	ARG
23	21	35	THR
23	21	40	ARG
23	21	83	GLU
24	22	28	LYS
24	22	54	LYS
24	22	70	GLN
25	23	24	LYS
25	23	31	LEU
25	23	34	GLU
26	24	13	ARG
26	24	20	ASN
26	24	37	SER
26	24	48	ARG
26	24	61	ARG
26	24	62	ARG
27	25	33	CYS
27	25	40	LYS
27	25	55	ARG

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Mol	Chain	Res	Type
28	26	6	ARG
28	26	13	CYS
28	26	19	ARG
28	26	20	ASN
28	26	34	LEU
28	26	40	CYS
28	26	50	ARG
29	27	1	MET
29	27	43	THR
29	27	48	LYS
30	28	14	VAL
30	28	31	HIS
30	28	34	TRP
30	28	37	SER
30	28	48	PHE
31	29	28	GLU
33	2b	7	VAL
33	2b	8	LYS
33	2b	9	GLU
33	2b	16	HIS
33	2b	24	TRP
33	2b	28	PHE
33	2b	35	GLU
33	2b	67	THR
33	2b	68	ILE
33	2b	71	VAL
33	2b	76	GLN
33	2b	80	ILE
33	2b	94	ASN
33	2b	107	THR
33	2b	112	VAL
33	2b	138	LEU
33	2b	144	ARG
33	2b	153	ARG
33	2b	157	ARG
33	2b	185	ILE
33	2b	189	ASP
33	2b	212	GLN
33	2b	220	ASP
34	2c	4	LYS
34	2c	15	THR
34	2c	16	ARG

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Mol	Chain	Res	Type
34	2c	18	TRP
34	2c	35	GLU
34	2c	47	LEU
34	2c	70	VAL
34	2c	89	GLU
34	2c	105	GLU
34	2c	119	ARG
34	2c	120	VAL
34	2c	142	MET
34	2c	192	THR
35	2d	8	VAL
35	2d	31	CYS
35	2d	34	GLU
35	2d	47	ARG
35	2d	58	LEU
35	2d	73	ARG
35	2d	86	LYS
35	2d	135	LEU
35	2d	150	GLU
35	2d	155	LEU
35	2d	156	GLU
35	2d	169	LYS
35	2d	175	SER
35	2d	201	GLN
36	2e	5	ASP
36	2e	13	ILE
36	2e	20	GLN
36	2e	24	ARG
36	2e	25	ARG
36	2e	31	LEU
36	2e	41	VAL
36	2e	51	VAL
36	2e	55	VAL
36	2e	75	THR
36	2e	78	HIS
36	2e	87	SER
36	2e	121	LYS
36	2e	125	SER
36	2e	151	LEU
37	2f	21	LEU
37	2f	31	GLU
37	2f	63	TYR

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Mol	Chain	Res	Type
37	2f	69	GLU
37	2f	70	ASP
37	2f	72	VAL
38	2g	4	ARG
38	2g	9	VAL
38	2g	51	GLN
38	2g	59	LEU
38	2g	75	VAL
38	2g	78	ARG
38	2g	79	ARG
38	2g	85	TYR
38	2g	92	SER
38	2g	146	GLU
39	2h	24	THR
39	2h	25	ASP
39	2h	39	LEU
39	2h	51	VAL
39	2h	52	ASP
39	2h	81	HIS
39	2h	109	ILE
39	2h	112	LEU
39	2h	122	ARG
39	2h	127	LEU
40	2i	17	VAL
40	2i	29	ASN
40	2i	32	ASP
40	2i	38	GLN
40	2i	54	ASP
40	2i	65	VAL
40	2i	92	TYR
40	2i	99	LEU
40	2i	102	LEU
40	2i	114	TYR
40	2i	125	TYR
40	2i	128	ARG
41	2j	13	HIS
41	2j	21	GLN
41	2j	33	GLN
41	2j	35	SER
41	2j	46	ARG
41	2j	67	THR
41	2j	73	ASP

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Mol	Chain	Res	Type
41	2j	74	ILE
41	2j	95	GLU
42	2k	14	VAL
42	2k	25	TYR
42	2k	28	THR
42	2k	33	THR
42	2k	57	THR
42	2k	62	GLN
42	2k	107	SER
42	2k	116	HIS
42	2k	117	ASN
43	2l	6	THR
43	2l	18	VAL
43	2l	33	ARG
43	2l	40	VAL
43	2l	53	ARG
43	2l	54	LYS
43	2l	81	SER
43	2l	116	SER
44	2m	4	ILE
44	2m	20	THR
44	2m	32	GLU
44	2m	44	ARG
44	2m	49	THR
44	2m	73	GLU
44	2m	102	ARG
44	2m	105	THR
44	2m	106	ASN
45	2n	3	ARG
45	2n	11	LYS
45	2n	32	SER
45	2n	33	VAL
45	2n	41	ARG
45	2n	56	VAL
46	2o	54	ARG
46	2o	76	GLU
47	2p	1	MET
47	2p	2	VAL
47	2p	11	SER
47	2p	21	VAL
47	2p	72	ARG
47	2p	73	LEU

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Mol	Chain	Res	Type
48	2q	5	VAL
48	2q	53	LEU
48	2q	83	ASP
48	2q	99	SER
49	2r	25	THR
49	2r	37	VAL
49	2r	63	GLN
49	2r	65	ILE
50	2s	12	ASP
50	2s	20	LEU
50	2s	27	GLU
50	2s	41	VAL
50	2s	49	ILE
50	2s	79	THR
51	2t	8	ARG
51	2t	9	ASN
51	2t	15	ARG
51	2t	45	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (124) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	164	GLN
4	1E	48	GLN
5	1F	69	HIS
5	1F	203	GLN
6	1G	26	GLN
7	1H	74	ASN
8	1I	133	HIS
8	1I	139	GLN
10	1O	3	GLN
12	1Q	12	GLN
12	1Q	57	HIS
12	1Q	123	HIS
14	1S	38	GLN
14	1S	68	GLN
14	1S	95	HIS
15	1T	58	ASN
16	1U	81	HIS
16	1U	94	ASN
19	1X	31	HIS
19	1X	82	GLN

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Mol	Chain	Res	Type
21	1Z	32	HIS
21	1Z	34	ASN
24	12	65	ASN
33	1b	37	ASN
33	1b	40	HIS
33	1b	45	GLN
33	1b	78	GLN
34	1c	6	HIS
34	1c	28	GLN
34	1c	37	GLN
34	1c	162	GLN
34	1c	170	GLN
35	1d	77	ASN
35	1d	116	GLN
35	1d	123	HIS
35	1d	160	GLN
36	1e	20	GLN
36	1e	78	HIS
37	1f	18	GLN
37	1f	57	GLN
37	1f	73	ASN
37	1f	100	ASN
38	1g	28	ASN
40	1i	3	GLN
40	1i	31	GLN
40	1i	34	ASN
40	1i	89	ASN
40	1i	124	GLN
41	1j	56	HIS
42	1k	62	GLN
42	1k	93	GLN
44	1m	92	HIS
44	1m	106	ASN
46	1o	46	HIS
47	1p	13	HIS
47	1p	76	GLN
48	1q	93	GLN
49	1r	63	GLN
50	1s	23	ASN
50	1s	47	HIS
50	1s	57	HIS
50	1s	83	HIS

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Mol	Chain	Res	Type
51	1t	90	GLN
3	2D	87	ASN
4	2E	48	GLN
5	2F	69	HIS
5	2F	160	ASN
7	2H	139	GLN
8	2I	139	GLN
10	2O	3	GLN
10	2O	5	GLN
12	2Q	12	GLN
12	2Q	123	HIS
14	2S	38	GLN
15	2T	43	GLN
15	2T	58	ASN
15	2T	84	GLN
19	2X	31	HIS
21	2Z	32	HIS
21	2Z	73	GLN
22	20	50	ASN
24	22	9	GLN
24	22	65	ASN
25	23	32	GLN
33	2b	45	GLN
33	2b	94	ASN
33	2b	95	GLN
33	2b	110	GLN
33	2b	146	GLN
34	2c	6	HIS
34	2c	162	GLN
34	2c	170	GLN
34	2c	181	ASN
35	2d	116	GLN
35	2d	123	HIS
35	2d	125	HIS
35	2d	201	GLN
36	2e	20	GLN
37	2f	100	ASN
38	2g	28	ASN
38	2g	68	ASN
38	2g	86	GLN
40	2i	3	GLN
40	2i	58	HIS

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Mol	Chain	Res	Type
40	2i	87	GLN
40	2i	89	ASN
41	2j	13	HIS
41	2j	21	GLN
42	2k	22	HIS
42	2k	38	ASN
42	2k	78	GLN
42	2k	104	GLN
42	2k	117	ASN
43	2l	99	HIS
44	2m	40	ASN
44	2m	62	ASN
44	2m	77	ASN
47	2p	13	HIS
48	2q	26	GLN
48	2q	93	GLN
49	2r	63	GLN
50	2s	69	HIS
51	2t	18	GLN
51	2t	75	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2863/2915 (98%)	426 (14%)	27 (0%)
1	2A	2790/2915 (95%)	450 (16%)	24 (0%)
2	1B	119/121 (98%)	10 (8%)	0
2	2B	118/121 (97%)	25 (21%)	0
32	1a	1494/1521 (98%)	247 (16%)	0
32	2a	1498/1521 (98%)	275 (18%)	0
53	1v	12/24 (50%)	3 (25%)	0
53	2v	12/24 (50%)	3 (25%)	0
54	1w	70/74 (94%)	25 (35%)	0
54	2w	68/74 (91%)	27 (39%)	0
55	1x	75/77 (97%)	7 (9%)	0
55	2x	75/77 (97%)	7 (9%)	0
57	1y	71/74 (95%)	28 (39%)	0
57	2y	71/74 (95%)	33 (46%)	0
All	All	9336/9612 (97%)	1566 (16%)	51 (0%)

All (1566) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	11	G
1	1A	12	U
1	1A	34	C
1	1A	45	C
1	1A	71	A
1	1A	74	A
1	1A	75	G
1	1A	84	A
1	1A	95	G
1	1A	118	A
1	1A	119	A
1	1A	120	U
1	1A	182	A
1	1A	196	A
1	1A	205	G
1	1A	215	G
1	1A	216	A
1	1A	221	A
1	1A	222	A
1	1A	225	A
1	1A	229	A
1	1A	232	G
1	1A	233	A
1	1A	248	G
1	1A	269	U
1	1A	271(C)	C
1	1A	271(K)	U
1	1A	271(L)	U
1	1A	271(M)	G
1	1A	271(N)	U
1	1A	271(S)	G
1	1A	272(B)	G
1	1A	272(G)	C
1	1A	272(H)	C
1	1A	272(I)	U
1	1A	275	G
1	1A	279	C
1	1A	311	A
1	1A	329	G
1	1A	330	A
1	1A	352	G
1	1A	363	G
1	1A	363(B)	G

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Mol	Chain	Res	Type
1	1A	370	G
1	1A	380	U
1	1A	386	G
1	1A	396	G
1	1A	405	U
1	1A	411	G
1	1A	412	A
1	1A	421	U
1	1A	428	A
1	1A	444	C
1	1A	448	U
1	1A	455	C
1	1A	456	C
1	1A	457	A
1	1A	467	G
1	1A	481	G
1	1A	504	U
1	1A	505	A
1	1A	509	C
1	1A	512	G
1	1A	528	A
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	587	C
1	1A	592	G
1	1A	603	A
1	1A	604	G
1	1A	607	U
1	1A	614(B)	G
1	1A	615	G
1	1A	616	G
1	1A	627	A
1	1A	637	A
1	1A	645	C

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Mol	Chain	Res	Type
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	740	U
1	1A	764	A
1	1A	775	G
1	1A	776	G
1	1A	782	A
1	1A	784	A
1	1A	785	G
1	1A	790	C
1	1A	792	G
1	1A	805	G
1	1A	812	C
1	1A	819	A
1	1A	827	U
1	1A	828	U
1	1A	859	G
1	1A	866	A
1	1A	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	895	U
1	1A	896	A
1	1A	897	C
1	1A	898	C
1	1A	907	U
1	1A	910	A
1	1A	931	G

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Mol	Chain	Res	Type
1	1A	932	G
1	1A	945	A
1	1A	946	G
1	1A	959	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	1041	C
1	1A	1044	G
1	1A	1045	A
1	1A	1046	A
1	1A	1047	G
1	1A	1054	A
1	1A	1055	G
1	1A	1058	G
1	1A	1063	G
1	1A	1066	U
1	1A	1070	A
1	1A	1071	G
1	1A	1073	A
1	1A	1075	C
1	1A	1076	C
1	1A	1078	U
1	1A	1079	C
1	1A	1083	U
1	1A	1087	G
1	1A	1088	A
1	1A	1090	U
1	1A	1091	G
1	1A	1093	G
1	1A	1094	U
1	1A	1096	A
1	1A	1097	U

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Mol	Chain	Res	Type
1	1A	1098	A
1	1A	1101	U
1	1A	1109	C
1	1A	1110	G
1	1A	1111	A
1	1A	1112	G
1	1A	1115	G
1	1A	1116	C
1	1A	1128	A
1	1A	1135	C
1	1A	1136	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
1	1A	1178	C
1	1A	1220	A
1	1A	1244	G
1	1A	1253	A
1	1A	1256	G
1	1A	1271	G
1	1A	1272	A
1	1A	1273	U
1	1A	1300	U
1	1A	1301	A
1	1A	1303	G
1	1A	1308	A
1	1A	1352	U
1	1A	1359	A
1	1A	1360	A
1	1A	1365	A
1	1A	1370	C
1	1A	1380	G
1	1A	1384	A
1	1A	1385	G
1	1A	1396	U
1	1A	1416	G
1	1A	1417	C
1	1A	1420	U

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Mol	Chain	Res	Type
1	1A	1421	G
1	1A	1428	C
1	1A	1437	C
1	1A	1445	A
1	1A	1450	G
1	1A	1455	G
1	1A	1467	C
1	1A	1482	G
1	1A	1490	A
1	1A	1493	C
1	1A	1508	A
1	1A	1509	C
1	1A	1509(A)	A
1	1A	1532	C
1	1A	1543	C
1	1A	1554	A
1	1A	1558	A
1	1A	1566	A
1	1A	1569	A
1	1A	1578	U
1	1A	1580	A
1	1A	1581	G
1	1A	1582	C
1	1A	1584	C
1	1A	1586	A
1	1A	1608	A
1	1A	1610	A
1	1A	1647	G
1	1A	1648	C
1	1A	1654	A
1	1A	1674	G
1	1A	1696	G
1	1A	1700	A
1	1A	1701	A
1	1A	1703	G
1	1A	1722	A
1	1A	1756	G
1	1A	1758	G
1	1A	1763	G
1	1A	1764	G
1	1A	1773	A
1	1A	1780	A

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Mol	Chain	Res	Type
1	1A	1782	C
1	1A	1791	A
1	1A	1800	C
1	1A	1801	G
1	1A	1816	G
1	1A	1828	G
1	1A	1829	A
1	1A	1847	A
1	1A	1878	G
1	1A	1889	A
1	1A	1900	A
1	1A	1906	G
1	1A	1927	A
1	1A	1929	G
1	1A	1930	G
1	1A	1937	A
1	1A	1938	A
1	1A	1955	U
1	1A	1963	U
1	1A	1965	C
1	1A	1967	C
1	1A	1970	A
1	1A	1971	A
1	1A	1972	A
1	1A	1992	G
1	1A	1993	U
1	1A	1997	G
1	1A	2020	A
1	1A	2023	G
1	1A	2031	A
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	2093	G
1	1A	2102	U
1	1A	2113	U
1	1A	2114	A

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Mol	Chain	Res	Type
1	1A	2116	G
1	1A	2118	U
1	1A	2119	A
1	1A	2120	G
1	1A	2121	G
1	1A	2123	G
1	1A	2126	A
1	1A	2127	G
1	1A	2129	C
1	1A	2131	G
1	1A	2132	U
1	1A	2133	G
1	1A	2134	A
1	1A	2135	A
1	1A	2136	C
1	1A	2142	C
1	1A	2143	C
1	1A	2144	U
1	1A	2146	C
1	1A	2147	G
1	1A	2148	G
1	1A	2150	U
1	1A	2151	G
1	1A	2155	G
1	1A	2156	G
1	1A	2157	G
1	1A	2158	A
1	1A	2159	G
1	1A	2161	C
1	1A	2162	G
1	1A	2165	G
1	1A	2166	G
1	1A	2167	U
1	1A	2169	A
1	1A	2172	U
1	1A	2173	A
1	1A	2174	C
1	1A	2181	G
1	1A	2182	G
1	1A	2183	C
1	1A	2184	G
1	1A	2189	U

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Mol	Chain	Res	Type
1	1A	2190	G
1	1A	2192	G
1	1A	2198	A
1	1A	2206	G
1	1A	2207	G
1	1A	2208	A
1	1A	2225	A
1	1A	2238	G
1	1A	2239	G
1	1A	2267	A
1	1A	2268	A
1	1A	2269	A
1	1A	2283	C
1	1A	2286	A
1	1A	2287	A
1	1A	2305	A
1	1A	2308	G
1	1A	2320	A
1	1A	2325	G
1	1A	2334	G
1	1A	2336	A
1	1A	2347	C
1	1A	2350	C
1	1A	2354	G
1	1A	2361	A
1	1A	2372	G
1	1A	2379	G
1	1A	2383	G
1	1A	2385	C
1	1A	2406	U
1	1A	2422	A
1	1A	2423	U
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

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Mol	Chain	Res	Type
1	1A	2478	A
1	1A	2490	G
1	1A	2491	U
1	1A	2502	G
1	1A	2505	G
1	1A	2518	A
1	1A	2529	G
1	1A	2554	U
1	1A	2566	A
1	1A	2567	G
1	1A	2573	C
1	1A	2602	A
1	1A	2611	U
1	1A	2612	C
1	1A	2629	A
1	1A	2630	G
1	1A	2641	G
1	1A	2654	A
1	1A	2689	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	2764	A
1	1A	2765	A
1	1A	2766	G
1	1A	2769	C
1	1A	2778	A
1	1A	2790	A
1	1A	2791	C
1	1A	2793	G
1	1A	2794	C
1	1A	2802	G
1	1A	2805	G
1	1A	2820	A
1	1A	2821	A
1	1A	2835	A
1	1A	2858	C

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Mol	Chain	Res	Type
1	1A	2872	G
1	1A	2880	C
1	1A	2893	G
1	1A	2894	G
1	1A	2895	U
2	1B	2	C
2	1B	13	A
2	1B	35	U
2	1B	45	A
2	1B	50	G
2	1B	56	G
2	1B	73	A
2	1B	84	C
2	1B	85	G
2	1B	110	G
32	1a	7	G
32	1a	9	G
32	1a	22	G
32	1a	32	A
32	1a	33	A
32	1a	39	G
32	1a	48	C
32	1a	50	A
32	1a	51	A
32	1a	54	C
32	1a	61	G
32	1a	76	C
32	1a	78	G
32	1a	79	G
32	1a	91	C
32	1a	96	U
32	1a	97	G
32	1a	98	G
32	1a	101	A
32	1a	116	A
32	1a	121	C
32	1a	131	C
32	1a	162	A
32	1a	163	C
32	1a	174	C
32	1a	180	U
32	1a	182	U

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Mol	Chain	Res	Type
32	1a	189(F)	U
32	1a	189(H)	G
32	1a	195	A
32	1a	197	A
32	1a	203	U
32	1a	204	U
32	1a	222	U
32	1a	247	G
32	1a	251	G
32	1a	266	G
32	1a	267	C
32	1a	279	A
32	1a	289	G
32	1a	306	G
32	1a	321	A
32	1a	328	C
32	1a	329	A
32	1a	332	G
32	1a	347	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	397	A
32	1a	398	C
32	1a	406	G
32	1a	412	A
32	1a	413	G
32	1a	422	C
32	1a	423	G
32	1a	424	G
32	1a	429	U
32	1a	439	A
32	1a	452	A
32	1a	461	A
32	1a	470	C
32	1a	471	G
32	1a	480	U
32	1a	482	A

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Mol	Chain	Res	Type
32	1a	483	C
32	1a	485	G
32	1a	493	G
32	1a	495	A
32	1a	496	A
32	1a	498	U
32	1a	505	G
32	1a	509	A
32	1a	510	A
32	1a	511	C
32	1a	518	C
32	1a	521	G
32	1a	524	G
32	1a	531	U
32	1a	532	A
32	1a	533	A
32	1a	536	C
32	1a	547	A
32	1a	550	G
32	1a	559	A
32	1a	560	U
32	1a	561	U
32	1a	568	G
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	577	G
32	1a	592	G
32	1a	596	C
32	1a	627	G
32	1a	630	G
32	1a	653	A
32	1a	665	A
32	1a	672	U
32	1a	673	G
32	1a	687	A
32	1a	688	G
32	1a	693	G
32	1a	695	A
32	1a	703	G
32	1a	723	U
32	1a	724	G

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Mol	Chain	Res	Type
32	1a	731	G
32	1a	747	C
32	1a	749	C
32	1a	755	G
32	1a	777	A
32	1a	793	U
32	1a	794	A
32	1a	815	A
32	1a	817	C
32	1a	828	A
32	1a	840	C
32	1a	841	U
32	1a	851	G
32	1a	891	U
32	1a	902	G
32	1a	914	A
32	1a	922	G
32	1a	926	G
32	1a	927	G
32	1a	934	C
32	1a	935	A
32	1a	942	G
32	1a	958	A
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	989	C
32	1a	992	U
32	1a	993	G
32	1a	996	A
32	1a	997	U
32	1a	1000	U
32	1a	1003	G
32	1a	1004	A
32	1a	1005	A

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Mol	Chain	Res	Type
32	1a	1008	C
32	1a	1009	G
32	1a	1011	G
32	1a	1017	G
32	1a	1020	U
32	1a	1021	G
32	1a	1022	G
32	1a	1023	G
32	1a	1026	G
32	1a	1027	C
32	1a	1028	C
32	1a	1029	C
32	1a	1030(A)	G
32	1a	1030(C)	G
32	1a	1031	G
32	1a	1039	C
32	1a	1043	C
32	1a	1044	A
32	1a	1045	C
32	1a	1065	U
32	1a	1068	G
32	1a	1081	G
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1123	A
32	1a	1125	U
32	1a	1127	G
32	1a	1132	C
32	1a	1134	G
32	1a	1138	G
32	1a	1139	G
32	1a	1146	A
32	1a	1152	A
32	1a	1154	G
32	1a	1157	A
32	1a	1159	U
32	1a	1184	G
32	1a	1193	G
32	1a	1196	U
32	1a	1197	G
32	1a	1201	A

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Mol	Chain	Res	Type
32	1a	1202	G
32	1a	1213	A
32	1a	1214	C
32	1a	1222	G
32	1a	1227	A
32	1a	1236	A
32	1a	1238	A
32	1a	1250	A
32	1a	1253	G
32	1a	1256	A
32	1a	1257	U
32	1a	1258	G
32	1a	1260	C
32	1a	1270	C
32	1a	1275	A
32	1a	1278	U
32	1a	1279	A
32	1a	1280	A
32	1a	1286	A
32	1a	1287	A
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1319	A
32	1a	1320	C
32	1a	1323	G
32	1a	1338	G
32	1a	1340	A
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1364	U
32	1a	1370	G
32	1a	1397	C
32	1a	1419	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1446	U
32	1a	1447	A
32	1a	1452	C
32	1a	1456	G
32	1a	1487	G

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Mol	Chain	Res	Type
32	1a	1492	A
32	1a	1494	G
32	1a	1497	G
32	1a	1503	A
32	1a	1504	G
32	1a	1505	G
32	1a	1506	U
32	1a	1517	G
32	1a	1529	G
32	1a	1530	G
53	1v	13	A
53	1v	14	A
53	1v	15	A
54	1w	2	C
54	1w	5	G
54	1w	8	4SU
54	1w	9	A
54	1w	14	A
54	1w	15	A
54	1w	18	G
54	1w	19	U
54	1w	21	A
54	1w	23	A
54	1w	24	A
54	1w	27	A
54	1w	45	U
54	1w	46	A
54	1w	48	C
54	1w	49	G
54	1w	50	A
54	1w	56	C
54	1w	62	C
54	1w	66	C
54	1w	67	G
54	1w	70	C
54	1w	71	G
54	1w	73	U
54	1w	74	C
55	1x	2	G
55	1x	9	G
55	1x	18	G
55	1x	19	G

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Mol	Chain	Res	Type
55	1x	20	U
55	1x	47	U
55	1x	61	C
57	1y	4	G
57	1y	5	G
57	1y	7	G
57	1y	9	A
57	1y	14	A
57	1y	18	G
57	1y	19	U
57	1y	21	A
57	1y	33	U
57	1y	34	C
57	1y	35	C
57	1y	39	G
57	1y	41	U
57	1y	44	A
57	1y	45	U
57	1y	46	A
57	1y	48	C
57	1y	49	G
57	1y	50	A
57	1y	51	G
57	1y	57	G
57	1y	58	A
57	1y	59	U
57	1y	65	U
57	1y	66	C
57	1y	69	C
57	1y	70	C
57	1y	71	G
1	2A	15	G
1	2A	34	C
1	2A	35	G
1	2A	45	C
1	2A	61	G
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	84	A
1	2A	90	U
1	2A	95	G

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Mol	Chain	Res	Type
1	2A	100	G
1	2A	102	G
1	2A	118	A
1	2A	119	A
1	2A	120	U
1	2A	140	G
1	2A	141	A
1	2A	154(A)	C
1	2A	157	U
1	2A	172	C
1	2A	173	G
1	2A	196	A
1	2A	199	A
1	2A	205	G
1	2A	215	G
1	2A	216	A
1	2A	222	A
1	2A	228	A
1	2A	229	A
1	2A	230	U
1	2A	232	G
1	2A	233	A
1	2A	248	G
1	2A	250	G
1	2A	266	G
1	2A	271(J)	C
1	2A	271(K)	U
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	271(O)	C
1	2A	272	G
1	2A	272(B)	G
1	2A	274	G
1	2A	277	C
1	2A	278	A
1	2A	311	A
1	2A	312	G
1	2A	324	A
1	2A	326	G
1	2A	327	G
1	2A	329	G

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Mol	Chain	Res	Type
1	2A	330	A
1	2A	352	G
1	2A	363	G
1	2A	363(B)	G
1	2A	386	G
1	2A	396	G
1	2A	399	G
1	2A	405	U
1	2A	411	G
1	2A	412	A
1	2A	422	A
1	2A	443	A
1	2A	444	C
1	2A	455	C
1	2A	456	C
1	2A	457	A
1	2A	481	G
1	2A	504	U
1	2A	505	A
1	2A	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	563	G
1	2A	573	G
1	2A	575	A
1	2A	586	A
1	2A	588	U
1	2A	599	G
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	614(B)	G
1	2A	615	G
1	2A	627	A
1	2A	637	A
1	2A	645	C
1	2A	652(B)	A
1	2A	652(C)	G

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Mol	Chain	Res	Type
1	2A	653	A
1	2A	669	G
1	2A	686	G
1	2A	717	G
1	2A	730	C
1	2A	752	A
1	2A	753	C
1	2A	764	A
1	2A	775	G
1	2A	776	G
1	2A	782	A
1	2A	784	A
1	2A	785	G
1	2A	792	G
1	2A	805	G
1	2A	812	C
1	2A	819	A
1	2A	827	U
1	2A	828	U
1	2A	832	G
1	2A	847	U
1	2A	857	C
1	2A	859	G
1	2A	866	A
1	2A	867	C
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	892	G
1	2A	893	C
1	2A	894	C
1	2A	896	A
1	2A	897	C
1	2A	899	A
1	2A	900	A
1	2A	901	A

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Mol	Chain	Res	Type
1	2A	910	A
1	2A	915	C
1	2A	917	A
1	2A	932	G
1	2A	938	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	1012	U
1	2A	1013	C
1	2A	1017	G
1	2A	1020	A
1	2A	1022	G
1	2A	1033	U
1	2A	1038	C
1	2A	1039	G
1	2A	1041	C
1	2A	1043	C
1	2A	1117	G
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1139	G
1	2A	1169	G
1	2A	1170	G
1	2A	1171	G
1	2A	1188	U
1	2A	1195	G
1	2A	1211	U
1	2A	1219	G
1	2A	1220	A
1	2A	1236	G
1	2A	1240	U
1	2A	1244	G
1	2A	1253	A

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Mol	Chain	Res	Type
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A
1	2A	1273	U
1	2A	1287	A
1	2A	1300	U
1	2A	1301	A
1	2A	1303	G
1	2A	1314	C
1	2A	1321	A
1	2A	1342	A
1	2A	1345	C
1	2A	1352	U
1	2A	1359	A
1	2A	1360	A
1	2A	1365	A
1	2A	1368	G
1	2A	1370	C
1	2A	1380	G
1	2A	1384	A
1	2A	1385	G
1	2A	1416	G
1	2A	1417	C
1	2A	1421	G
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	1459	G
1	2A	1460	A
1	2A	1461	G
1	2A	1467	C
1	2A	1471	A
1	2A	1478	G
1	2A	1482	G
1	2A	1490	A
1	2A	1493	C
1	2A	1494	A
1	2A	1496	A
1	2A	1497	U

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Mol	Chain	Res	Type
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1531	C
1	2A	1532	C
1	2A	1542	A
1	2A	1543	C
1	2A	1547	C
1	2A	1558	A
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1580	A
1	2A	1583	A
1	2A	1584	C
1	2A	1608	A
1	2A	1609	A
1	2A	1610	A
1	2A	1648	C
1	2A	1654	A
1	2A	1674	G
1	2A	1696	G
1	2A	1700	A
1	2A	1721	G
1	2A	1722	A
1	2A	1740	G
1	2A	1746	G
1	2A	1756	G
1	2A	1758	G
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	1839	G

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Mol	Chain	Res	Type
1	2A	1847	A
1	2A	1848	A
1	2A	1877	A
1	2A	1878	G
1	2A	1884	A
1	2A	1900	A
1	2A	1906	G
1	2A	1914	C
1	2A	1929	G
1	2A	1930	G
1	2A	1936	A
1	2A	1937	A
1	2A	1938	A
1	2A	1955	U
1	2A	1963	U
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1992	G
1	2A	1993	U
1	2A	1997	G
1	2A	2020	A
1	2A	2023	G
1	2A	2030	A
1	2A	2031	A
1	2A	2032	G
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	2099	U
1	2A	2102	U
1	2A	2110	G
1	2A	2111	C
1	2A	2112	G
1	2A	2116	G
1	2A	2117	A
1	2A	2118	U

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Mol	Chain	Res	Type
1	2A	2120	G
1	2A	2122	U
1	2A	2125	G
1	2A	2126	A
1	2A	2127	G
1	2A	2128	C
1	2A	2129	C
1	2A	2131	G
1	2A	2132	U
1	2A	2133	G
1	2A	2134	A
1	2A	2135	A
1	2A	2136	C
1	2A	2137	C
1	2A	2138	C
1	2A	2140	C
1	2A	2142	C
1	2A	2143	C
1	2A	2145	C
1	2A	2146	C
1	2A	2148	G
1	2A	2149	G
1	2A	2150	U
1	2A	2151	G
1	2A	2156	G
1	2A	2157	G
1	2A	2158	A
1	2A	2159	G
1	2A	2161	C
1	2A	2165	G
1	2A	2166	G
1	2A	2167	U
1	2A	2168	G
1	2A	2172	U
1	2A	2173	A
1	2A	2174	C
1	2A	2176	A
1	2A	2178	C
1	2A	2188	C
1	2A	2189	U
1	2A	2192	G
1	2A	2198	A

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Mol	Chain	Res	Type
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2218	U
1	2A	2225	A
1	2A	2234	G
1	2A	2238	G
1	2A	2239	G
1	2A	2268	A
1	2A	2269	A
1	2A	2275	C
1	2A	2278	A
1	2A	2283	C
1	2A	2287	A
1	2A	2305	A
1	2A	2308	G
1	2A	2309	A
1	2A	2311	A
1	2A	2312	U
1	2A	2319	G
1	2A	2320	A
1	2A	2325	G
1	2A	2329	G
1	2A	2334	G
1	2A	2336	A
1	2A	2347	C
1	2A	2350	C
1	2A	2354	G
1	2A	2376	A
1	2A	2383	G
1	2A	2385	C
1	2A	2388	A
1	2A	2406	U
1	2A	2425	A
1	2A	2429	G
1	2A	2430	A
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2448	A
1	2A	2460	U
1	2A	2469	A

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Mol	Chain	Res	Type
1	2A	2474	C
1	2A	2476	A
1	2A	2478	A
1	2A	2487	G
1	2A	2491	U
1	2A	2502	G
1	2A	2505	G
1	2A	2506	U
1	2A	2507	C
1	2A	2518	A
1	2A	2520	C
1	2A	2525	G
1	2A	2529	G
1	2A	2535	G
1	2A	2549	G
1	2A	2554	U
1	2A	2555	U
1	2A	2566	A
1	2A	2567	G
1	2A	2573	C
1	2A	2585	U
1	2A	2602	A
1	2A	2611	U
1	2A	2612	C
1	2A	2615	U
1	2A	2630	G
1	2A	2634	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	2748	A
1	2A	2751	G
1	2A	2757	A
1	2A	2758	A
1	2A	2760	C

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Mol	Chain	Res	Type
1	2A	2764	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
1	2A	2804	C
1	2A	2805	G
1	2A	2818	G
1	2A	2820	A
1	2A	2821	A
1	2A	2835	A
1	2A	2839	G
1	2A	2872	G
1	2A	2880	C
1	2A	2894	G
1	2A	2897	U
2	2B	2	C
2	2B	8	U
2	2B	12	C
2	2B	13	A
2	2B	17	C
2	2B	19	G
2	2B	20	C
2	2B	25	A
2	2B	29	A
2	2B	34	U
2	2B	41	U
2	2B	42	C
2	2B	51	G
2	2B	53	A
2	2B	56	G
2	2B	73	A
2	2B	74	U
2	2B	75	G
2	2B	85	G
2	2B	88	C
2	2B	89	G
2	2B	91	C
2	2B	108	U

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Mol	Chain	Res	Type
2	2B	110	G
2	2B	120	A
32	2a	9	G
32	2a	22	G
32	2a	32	A
32	2a	39	G
32	2a	47	C
32	2a	48	C
32	2a	50	A
32	2a	51	A
32	2a	52	G
32	2a	66	G
32	2a	73	G
32	2a	80	G
32	2a	88	A
32	2a	89	C
32	2a	98	G
32	2a	101	A
32	2a	116	A
32	2a	121	C
32	2a	131	C
32	2a	143	A
32	2a	144	G
32	2a	159	G
32	2a	162	A
32	2a	163	C
32	2a	182	U
32	2a	189(F)	U
32	2a	195	A
32	2a	197	A
32	2a	202	U
32	2a	203	U
32	2a	204	U
32	2a	216	G
32	2a	217	C
32	2a	231	G
32	2a	247	G
32	2a	249	U
32	2a	250	A
32	2a	251	G
32	2a	266	G
32	2a	267	C

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Mol	Chain	Res	Type
32	2a	270	A
32	2a	289	G
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	344	A
32	2a	351	G
32	2a	352	C
32	2a	353	A
32	2a	354	G
32	2a	367	U
32	2a	372	C
32	2a	373	A
32	2a	384	G
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	412	A
32	2a	413	G
32	2a	421	U
32	2a	423	G
32	2a	429	U
32	2a	430	A
32	2a	439	A
32	2a	442	C
32	2a	452	A
32	2a	470	C
32	2a	471	G
32	2a	484	G
32	2a	485	G
32	2a	487	A
32	2a	496	A
32	2a	498	U
32	2a	499	A
32	2a	505	G
32	2a	509	A
32	2a	510	A
32	2a	511	C
32	2a	518	C
32	2a	521	G
32	2a	531	U
32	2a	532	A

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Mol	Chain	Res	Type
32	2a	533	A
32	2a	545	C
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	576	G
32	2a	577	G
32	2a	596	C
32	2a	597	G
32	2a	607	A
32	2a	619	U
32	2a	630	G
32	2a	653	A
32	2a	665	A
32	2a	666	G
32	2a	687	A
32	2a	688	G
32	2a	695	A
32	2a	705	U
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	774	G
32	2a	777	A
32	2a	792	A
32	2a	793	U
32	2a	794	A
32	2a	816	A
32	2a	817	C
32	2a	821	G
32	2a	828	A
32	2a	834	C
32	2a	836	G
32	2a	840	C
32	2a	841	U
32	2a	853	G

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Mol	Chain	Res	Type
32	2a	859	A
32	2a	874	G
32	2a	902	G
32	2a	914	A
32	2a	916	G
32	2a	926	G
32	2a	927	G
32	2a	931	C
32	2a	933	G
32	2a	934	C
32	2a	935	A
32	2a	958	A
32	2a	960	U
32	2a	961	U
32	2a	968	A
32	2a	969	A
32	2a	971	G
32	2a	972	C
32	2a	974	A
32	2a	975	A
32	2a	976	G
32	2a	977	A
32	2a	978	A
32	2a	989	C
32	2a	991	U
32	2a	992	U
32	2a	993	G
32	2a	995	C
32	2a	996	A
32	2a	997	U
32	2a	999	C
32	2a	1000	U
32	2a	1001	A
32	2a	1002	G
32	2a	1003	G
32	2a	1005	A
32	2a	1006	C
32	2a	1009	G
32	2a	1011	G
32	2a	1016	A
32	2a	1020	U
32	2a	1022	G

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Mol	Chain	Res	Type
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	1030(D)	A
32	2a	1032	G
32	2a	1033	G
32	2a	1034	G
32	2a	1035	A
32	2a	1039	C
32	2a	1040	U
32	2a	1051	C
32	2a	1053	G
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1077	G
32	2a	1078	U
32	2a	1079	G
32	2a	1081	G
32	2a	1086	U
32	2a	1092	A
32	2a	1094	G
32	2a	1095	U
32	2a	1101	A
32	2a	1108	G
32	2a	1109	C
32	2a	1113	C
32	2a	1122	U
32	2a	1125	U
32	2a	1126	U
32	2a	1127	G
32	2a	1129	C
32	2a	1130	A
32	2a	1133	G
32	2a	1135	U
32	2a	1136	U
32	2a	1137	C

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Mol	Chain	Res	Type
32	2a	1138	G
32	2a	1139	G
32	2a	1142	G
32	2a	1147	C
32	2a	1152	A
32	2a	1154	G
32	2a	1157	A
32	2a	1159	U
32	2a	1172	C
32	2a	1181	G
32	2a	1182	G
32	2a	1184	G
32	2a	1193	G
32	2a	1196	U
32	2a	1197	G
32	2a	1202	G
32	2a	1211	U
32	2a	1213	A
32	2a	1227	A
32	2a	1228	C
32	2a	1236	A
32	2a	1238	A
32	2a	1240	U
32	2a	1241	G
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	1279	A
32	2a	1280	A
32	2a	1286	A
32	2a	1287	A
32	2a	1299	A
32	2a	1302	U
32	2a	1303	C
32	2a	1305	G
32	2a	1312	G

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Mol	Chain	Res	Type
32	2a	1320	C
32	2a	1323	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	1398	A
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1446	U
32	2a	1452	C
32	2a	1456	G
32	2a	1492	A
32	2a	1497	G
32	2a	1504	G
32	2a	1506	U
32	2a	1507	A
32	2a	1517	G
32	2a	1529	G
32	2a	1530	G
32	2a	1531	A
32	2a	1532	U
53	2v	13	A
53	2v	14	A
53	2v	15	A
54	2w	6	C
54	2w	8	4SU
54	2w	9	A
54	2w	10	G
54	2w	12	U
54	2w	13	C
54	2w	14	A
54	2w	18	G
54	2w	22	G
54	2w	23	A
54	2w	24	A
54	2w	25	C
54	2w	26	G
54	2w	36	C

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Mol	Chain	Res	Type
54	2w	46	A
54	2w	48	C
54	2w	49	G
54	2w	50	A
54	2w	56	C
54	2w	57	G
54	2w	61	C
54	2w	62	C
54	2w	64	U
54	2w	69	C
54	2w	70	C
54	2w	72	C
54	2w	74	C
55	2x	3	C
55	2x	9	G
55	2x	19	G
55	2x	20	U
55	2x	21	A
55	2x	47	U
55	2x	48	C
57	2y	4	G
57	2y	5	G
57	2y	7	G
57	2y	8	4SU
57	2y	9	A
57	2y	15	A
57	2y	18	G
57	2y	19	U
57	2y	21	A
57	2y	22	G
57	2y	26	G
57	2y	27	A
57	2y	33	U
57	2y	34	C
57	2y	37	A
57	2y	45	U
57	2y	46	A
57	2y	48	C
57	2y	49	G
57	2y	52	G
57	2y	53	G
57	2y	55	PSU

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Mol	Chain	Res	Type
57	2y	57	G
57	2y	58	A
57	2y	59	U
57	2y	60	U
57	2y	61	C
57	2y	66	C
57	2y	67	G
57	2y	69	C
57	2y	70	C
57	2y	73	U
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(K)	U
1	1A	278	A
1	1A	548	A
1	1A	746	A
1	1A	774	A
1	1A	974	G
1	1A	1067	A
1	1A	1142(A)	A
1	1A	1174	A
1	1A	1176	G
1	1A	1379	A
1	1A	1442	G
1	1A	1508	A
1	1A	1608	A
1	1A	1762	A
1	1A	1992	G
1	1A	2126	A
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	2756	U

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Mol	Chain	Res	Type
1	2A	196	A
1	2A	228	A
1	2A	266	G
1	2A	271(K)	U
1	2A	271(M)	G
1	2A	277	C
1	2A	528	A
1	2A	752	A
1	2A	827	U
1	2A	856	C
1	2A	900	A
1	2A	1210	A
1	2A	1379	A
1	2A	1420	U
1	2A	1530	C
1	2A	1913	A
1	2A	1992	G
1	2A	2119	A
1	2A	2126	A
1	2A	2156	G
1	2A	2406	U
1	2A	2439	A
1	2A	2689	U
1	2A	2756	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
32	PSU	2a	516	32	18,21,22	1.32	2 (11%)	22,30,33	2.01	5 (22%)
1	5MU	1A	1915	1	19,22,23	1.42	4 (21%)	28,32,35	2.03	7 (25%)
54	4SU	1w	8	54	18,21,22	1.65	4 (22%)	26,30,33	2.16	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	UR3	1a	1498	32	19,22,23	0.99	1 (5%)	26,32,35	1.40	1 (3%)
57	5MU	1y	54	57	19,22,23	1.43	5 (26%)	28,32,35	1.99	6 (21%)
32	2MG	1a	1207	32,58	18,26,27	0.91	1 (5%)	16,38,41	1.05	1 (6%)
54	PSU	2w	55	58,54	18,21,22	1.34	2 (11%)	22,30,33	1.90	3 (13%)
1	OMC	2A	1920	1	19,22,23	0.81	0	26,31,34	0.90	1 (3%)
1	5MC	2A	1962	1,58	18,22,23	0.98	2 (11%)	26,32,35	1.19	2 (7%)
55	PSU	2x	55	55	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
54	L3X	1w	76	1,54	21,28,29	1.58	3 (14%)	15,40,43	1.62	1 (6%)
32	5MC	2a	1404	32	18,22,23	1.01	2 (11%)	26,32,35	1.16	3 (11%)
32	4OC	2a	1402	32,58	20,23,24	0.77	0	26,32,35	0.96	2 (7%)
54	L3X	2w	76	1,54	21,28,29	1.41	4 (19%)	15,40,43	1.58	1 (6%)
32	MA6	1a	1518	32	19,26,27	0.82	0	18,38,41	1.41	2 (11%)
1	5MU	2A	1939	1,58	19,22,23	1.43	5 (26%)	28,32,35	2.36	6 (21%)
32	MA6	1a	1519	32	19,26,27	0.82	0	18,38,41	1.47	2 (11%)
1	OMC	1A	1920	1	19,22,23	0.82	0	26,31,34	1.01	1 (3%)
1	OMU	2A	2552	1,58	19,22,23	1.22	3 (15%)	26,31,34	1.79	5 (19%)
32	5MC	1a	967	32	18,22,23	0.99	2 (11%)	26,32,35	1.16	2 (7%)
57	4SU	1y	8	57	18,21,22	1.69	5 (27%)	26,30,33	1.70	4 (15%)
1	PSU	1A	2605	1,58	18,21,22	1.35	3 (16%)	22,30,33	1.93	3 (13%)
32	5MC	1a	1407	32	18,22,23	0.98	2 (11%)	26,32,35	1.11	2 (7%)
32	MA6	2a	1518	32	19,26,27	0.82	0	18,38,41	1.33	2 (11%)
55	PSU	1x	55	55,58	18,21,22	1.31	2 (11%)	22,30,33	1.97	4 (18%)
55	4SU	1x	8	55	18,21,22	2.26	5 (27%)	26,30,33	1.84	6 (23%)
1	2MA	2A	2503	1,58	17,25,26	1.05	1 (5%)	17,37,40	0.93	2 (11%)
32	5MC	2a	967	32	18,22,23	0.93	2 (11%)	26,32,35	1.14	3 (11%)
32	5MC	2a	1407	32	18,22,23	0.96	2 (11%)	26,32,35	1.24	3 (11%)
55	4SU	2x	8	55	18,21,22	1.91	5 (27%)	26,30,33	1.42	4 (15%)
1	PSU	2A	1911	1	18,21,22	1.37	2 (11%)	22,30,33	1.80	3 (13%)
32	G7M	2a	527	32,58	20,26,27	1.30	2 (10%)	17,39,42	0.56	0
54	5MU	1w	54	54	19,22,23	1.39	4 (21%)	28,32,35	1.94	7 (25%)
1	5MC	2A	1942	1	18,22,23	0.99	2 (11%)	26,32,35	1.08	2 (7%)
56	FME	1z	1	56	8,9,10	1.00	0	7,9,11	0.92	0
32	UR3	2a	1498	32	19,22,23	1.01	0	26,32,35	1.45	2 (7%)
56	FME	2z	1	56	8,9,10	0.97	0	7,9,11	1.05	1 (14%)
57	PSU	2y	55	57	18,21,22	1.38	2 (11%)	22,30,33	1.88	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
43	0TD	1l	92	43	7,9,10	4.80	1 (14%)	6,11,13	4.48	2 (33%)
1	5MC	1A	1942	1	18,22,23	0.98	2 (11%)	26,32,35	1.23	3 (11%)
1	OMU	1A	2552	1,58	19,22,23	1.20	3 (15%)	26,31,34	1.78	6 (23%)
55	5MC	2x	32	55	18,22,23	1.00	2 (11%)	26,32,35	1.22	3 (11%)
32	2MG	2a	1207	32,58	18,26,27	0.93	1 (5%)	16,38,41	1.04	2 (12%)
55	8AN	1x	76	55,58	19,24,25	1.27	3 (15%)	13,35,38	1.89	2 (15%)
57	PSU	1y	55	57	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
1	2MA	1A	2503	1,58	17,25,26	1.07	2 (11%)	17,37,40	1.01	2 (11%)
32	4OC	1a	1402	32	20,23,24	0.75	0	26,32,35	0.93	1 (3%)
1	PSU	1A	1917	1	18,21,22	1.33	2 (11%)	22,30,33	1.88	3 (13%)
32	G7M	1a	527	32,58	20,26,27	1.21	2 (10%)	17,39,42	0.57	0
1	PSU	1A	1911	1	18,21,22	1.36	2 (11%)	22,30,33	1.83	4 (18%)
43	0TD	2l	92	43	7,9,10	4.91	1 (14%)	6,11,13	3.35	2 (33%)
32	PSU	1a	516	32	18,21,22	1.35	2 (11%)	22,30,33	1.91	4 (18%)
32	M2G	2a	966	32	20,27,28	1.42	3 (15%)	22,40,43	1.05	2 (9%)
32	M2G	1a	966	32	20,27,28	1.46	3 (15%)	22,40,43	0.96	2 (9%)
57	4SU	2y	8	57	18,21,22	1.64	5 (27%)	26,30,33	2.00	5 (19%)
1	OMG	2A	2251	55,1	18,26,27	0.92	1 (5%)	19,38,41	1.30	3 (15%)
32	MA6	2a	1519	32	19,26,27	0.81	0	18,38,41	1.55	2 (11%)
55	5MC	1x	32	55	18,22,23	1.04	2 (11%)	26,32,35	1.25	2 (7%)
1	5MC	1A	1962	1,58	18,22,23	0.94	2 (11%)	26,32,35	1.16	3 (11%)
55	5MU	2x	54	55	19,22,23	1.42	5 (26%)	28,32,35	1.94	5 (17%)
32	5MC	1a	1404	32	18,22,23	0.96	2 (11%)	26,32,35	1.16	3 (11%)
32	5MC	2a	1400	32	18,22,23	0.96	2 (11%)	26,32,35	1.19	3 (11%)
1	5MU	1A	1939	1,58	19,22,23	1.52	6 (31%)	28,32,35	2.02	5 (17%)
54	4SU	2w	8	54	18,21,22	1.73	5 (27%)	26,30,33	2.79	6 (23%)
1	5MU	2A	1915	1	19,22,23	1.41	5 (26%)	28,32,35	2.14	5 (17%)
55	8AN	2x	76	55,58	19,24,25	1.27	3 (15%)	13,35,38	1.86	2 (15%)
1	PSU	2A	2605	1	18,21,22	1.33	2 (11%)	22,30,33	2.07	4 (18%)
54	5MU	2w	54	54	19,22,23	1.40	4 (21%)	28,32,35	1.65	6 (21%)
1	OMG	1A	2251	55,1,58	18,26,27	1.03	1 (5%)	19,38,41	1.06	3 (15%)
57	5MU	2y	54	57	19,22,23	1.48	5 (26%)	28,32,35	1.86	7 (25%)
55	5MU	1x	54	55	19,22,23	1.45	6 (31%)	28,32,35	1.87	5 (17%)
54	PSU	1w	55	58,54	18,21,22	1.41	2 (11%)	22,30,33	1.91	4 (18%)
1	PSU	2A	1917	1	18,21,22	1.36	2 (11%)	22,30,33	1.93	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	5MC	1a	1400	32	18,22,23	0.97	2 (11%)	26,32,35	1.12	3 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
1	5MU	1A	1915	1	-	0/7/25/26	0/2/2/2
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
57	5MU	1y	54	57	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32,58	-	1/5/27/28	0/3/3/3
54	PSU	2w	55	58,54	-	0/7/25/26	0/2/2/2
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
1	5MC	2A	1962	1,58	-	0/7/25/26	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
54	L3X	1w	76	1,54	-	0/9/31/32	0/3/3/3
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32,58	-	2/9/29/30	0/2/2/2
54	L3X	2w	76	1,54	-	2/9/31/32	0/3/3/3
32	MA6	1a	1518	32	-	0/7/29/30	0/3/3/3
1	5MU	2A	1939	1,58	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	3/7/29/30	0/3/3/3
1	OMC	1A	1920	1	-	1/9/27/28	0/2/2/2
1	OMU	2A	2552	1,58	-	0/9/27/28	0/2/2/2
32	5MC	1a	967	32	-	2/7/25/26	0/2/2/2
57	4SU	1y	8	57	-	0/7/25/26	0/2/2/2
1	PSU	1A	2605	1,58	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	0/7/29/30	0/3/3/3
55	PSU	1x	55	55,58	-	0/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	1,58	-	1/3/25/26	0/3/3/3
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
55	4SU	2x	8	55	-	1/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
32	G7M	2a	527	32,58	-	2/3/25/26	0/3/3/3
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
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
56	FME	1z	1	56	-	3/7/9/11	-
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
56	FME	2z	1	56	-	0/7/9/11	-
57	PSU	2y	55	57	-	3/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	1/7/12/14	-
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
1	OMU	1A	2552	1,58	-	0/9/27/28	0/2/2/2
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32,58	-	1/5/27/28	0/3/3/3
55	8AN	1x	76	55,58	-	3/3/25/26	0/3/3/3
57	PSU	1y	55	57	-	2/7/25/26	0/2/2/2
1	2MA	1A	2503	1,58	-	2/3/25/26	0/3/3/3
32	4OC	1a	1402	32	-	1/9/29/30	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
32	G7M	1a	527	32,58	-	2/3/25/26	0/3/3/3
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	2/7/12/14	-
32	PSU	1a	516	32	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
57	4SU	2y	8	57	-	2/7/25/26	0/2/2/2
1	OMG	2A	2251	55,1	-	0/5/27/28	0/3/3/3
32	MA6	2a	1519	32	-	3/7/29/30	0/3/3/3
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
1	5MC	1A	1962	1,58	-	1/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	1,58	-	0/7/25/26	0/2/2/2
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
55	8AN	2x	76	55,58	-	3/3/25/26	0/3/3/3
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
1	OMG	1A	2251	55,1,58	-	0/5/27/28	0/3/3/3
57	5MU	2y	54	57	-	3/7/25/26	0/2/2/2
55	5MU	1x	54	55	-	0/7/25/26	0/2/2/2
54	PSU	1w	55	58,54	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2

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

All (174) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.66	1.69	1.82
43	1l	92	0TD	CB-SB	-12.34	1.69	1.82
55	1x	8	4SU	C4-N3	-5.73	1.31	1.37
32	1a	966	M2G	C2-N3	4.75	1.36	1.30
32	2a	966	M2G	C2-N3	4.50	1.36	1.30
54	2w	8	4SU	C4-S4	-4.50	1.59	1.68
55	1x	8	4SU	C4-S4	-4.44	1.60	1.68
54	1w	8	4SU	C4-S4	-4.31	1.60	1.68
55	2x	8	4SU	C4-N3	-4.27	1.33	1.37
57	2y	8	4SU	C4-S4	-4.22	1.60	1.68
57	1y	8	4SU	C4-S4	-4.14	1.60	1.68
54	1w	76	L3X	O4'-C1'	4.08	1.46	1.41
55	2x	8	4SU	C4-S4	-4.04	1.60	1.68
57	2y	55	PSU	C6-C5	3.99	1.40	1.35
55	1x	8	4SU	C2-N3	-3.96	1.30	1.38
54	1w	55	PSU	C6-C5	3.90	1.39	1.35
57	1y	55	PSU	C6-C5	3.75	1.39	1.35
32	2a	527	G7M	C5-C4	3.75	1.46	1.39
54	1w	76	L3X	C5-C4	-3.63	1.31	1.40
54	2w	55	PSU	C6-C5	3.62	1.39	1.35
32	1a	516	PSU	C6-C5	3.57	1.39	1.35
32	1a	527	G7M	C5-C4	3.55	1.46	1.39
55	2x	55	PSU	C6-C5	3.46	1.39	1.35
1	2A	1911	PSU	C6-C5	3.45	1.39	1.35
1	2A	1917	PSU	C6-C5	3.34	1.39	1.35
1	1A	1911	PSU	C6-C5	3.31	1.39	1.35
55	1x	8	4SU	C5-C4	-3.31	1.38	1.42
55	1x	55	PSU	C6-C5	3.26	1.39	1.35
32	2a	1404	5MC	C6-C5	3.19	1.39	1.34
54	2w	76	L3X	O4'-C1'	3.18	1.45	1.41
32	2a	516	PSU	C6-C5	3.15	1.39	1.35
54	2w	8	4SU	C2-N1	3.15	1.43	1.38
57	1y	8	4SU	C4-N3	-3.10	1.34	1.37
1	1A	1917	PSU	C6-C5	3.08	1.38	1.35
1	1A	1939	5MU	C4-N3	-3.06	1.33	1.38
1	1A	2605	PSU	C4-N3	-3.00	1.33	1.38
1	2A	1939	5MU	C6-C5	2.99	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2251	OMG	C6-N1	-2.96	1.33	1.37
1	2A	1942	5MC	C6-C5	2.96	1.39	1.34
55	1x	32	5MC	C6-C5	2.94	1.39	1.34
57	2y	54	5MU	C6-C5	2.94	1.39	1.34
1	2A	2605	PSU	C6-C5	2.94	1.38	1.35
32	1a	1407	5MC	C6-C5	2.91	1.39	1.34
32	1a	967	5MC	C6-C5	2.91	1.39	1.34
55	2x	54	5MU	C6-C5	2.91	1.39	1.34
55	1x	54	5MU	C6-C5	2.91	1.39	1.34
55	1x	76	8AN	C6-C5	-2.90	1.32	1.43
55	2x	8	4SU	C2-N3	-2.88	1.32	1.38
57	1y	54	5MU	C6-C5	2.86	1.39	1.34
1	2A	1939	5MU	C4-N3	-2.86	1.33	1.38
55	2x	32	5MC	C6-C5	2.86	1.39	1.34
1	1A	1915	5MU	C6-C5	2.85	1.39	1.34
1	1A	1939	5MU	C6-C5	2.83	1.39	1.34
55	1x	54	5MU	C4-N3	-2.82	1.33	1.38
54	2w	76	L3X	C5-C4	-2.81	1.33	1.40
32	1a	1400	5MC	C6-C5	2.79	1.39	1.34
1	2A	1915	5MU	C6-C5	2.79	1.39	1.34
55	2x	8	4SU	C5-C4	-2.79	1.39	1.42
1	1A	1942	5MC	C6-C5	2.76	1.39	1.34
1	1A	1962	5MC	C6-C5	2.76	1.39	1.34
55	1x	76	8AN	C5-C4	-2.75	1.33	1.40
55	2x	76	8AN	C5-C4	-2.75	1.33	1.40
32	2a	966	M2G	C2-N2	2.74	1.40	1.35
54	2w	54	5MU	C6-C5	2.73	1.39	1.34
57	2y	8	4SU	C4-N3	-2.72	1.34	1.37
54	1w	8	4SU	C5-C4	-2.71	1.39	1.42
1	2A	2605	PSU	C4-N3	-2.70	1.33	1.38
1	1A	1915	5MU	C2-N1	2.70	1.42	1.38
57	2y	54	5MU	C2-N1	2.69	1.42	1.38
57	2y	54	5MU	C4-N3	-2.69	1.33	1.38
32	2a	1400	5MC	C6-C5	2.68	1.39	1.34
54	1w	54	5MU	C6-C5	2.66	1.39	1.34
1	2A	2503	2MA	C2-N3	2.66	1.36	1.31
1	1A	1917	PSU	C4-N3	-2.66	1.33	1.38
1	2A	1917	PSU	C4-N3	-2.64	1.33	1.38
1	1A	1911	PSU	C4-N3	-2.64	1.33	1.38
32	2a	1407	5MC	C6-C5	2.63	1.38	1.34
55	2x	76	8AN	C6-C5	-2.60	1.33	1.43
54	1w	54	5MU	C2-N1	2.57	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1939	5MU	C4-C5	2.57	1.49	1.44
1	2A	1962	5MC	C6-C5	2.57	1.38	1.34
32	1a	516	PSU	C4-N3	-2.57	1.34	1.38
32	1a	1404	5MC	C6-C5	2.56	1.38	1.34
54	2w	8	4SU	C5-C4	-2.55	1.39	1.42
32	1a	966	M2G	C2-N2	2.55	1.40	1.35
55	2x	54	5MU	C4-N3	-2.55	1.34	1.38
32	1a	966	M2G	C6-N1	-2.54	1.34	1.37
54	2w	8	4SU	O2-C2	2.54	1.27	1.23
32	2a	527	G7M	C6-N1	-2.53	1.34	1.37
54	1w	54	5MU	C4-C5	2.52	1.49	1.44
1	2A	1911	PSU	C4-N3	-2.51	1.34	1.38
32	2a	967	5MC	C6-C5	2.51	1.38	1.34
32	2a	516	PSU	C4-N3	-2.51	1.34	1.38
1	2A	1962	5MC	C6-N1	-2.50	1.33	1.38
54	2w	76	L3X	C6-C5	-2.49	1.34	1.43
57	1y	54	5MU	C4-C5	2.49	1.48	1.44
1	1A	1915	5MU	C4-N3	-2.48	1.34	1.38
1	2A	1915	5MU	C4-C5	2.46	1.48	1.44
54	2w	54	5MU	C2-N1	2.46	1.42	1.38
54	1w	55	PSU	C4-N3	-2.46	1.34	1.38
32	1a	527	G7M	C6-N1	-2.45	1.34	1.37
57	2y	54	5MU	C4-C5	2.45	1.48	1.44
54	2w	54	5MU	C4-N3	-2.44	1.34	1.38
1	1A	1942	5MC	C6-N1	-2.44	1.33	1.38
1	2A	1915	5MU	C4-N3	-2.43	1.34	1.38
32	2a	966	M2G	C6-N1	-2.43	1.34	1.37
55	2x	55	PSU	C4-N3	-2.42	1.34	1.38
57	2y	8	4SU	C5-C4	-2.41	1.39	1.42
1	2A	1915	5MU	C2-N1	2.41	1.42	1.38
57	1y	54	5MU	C4-N3	-2.41	1.34	1.38
55	2x	54	5MU	C4-C5	2.41	1.48	1.44
57	1y	54	5MU	C2-N1	2.41	1.42	1.38
54	2w	55	PSU	C4-N3	-2.40	1.34	1.38
1	2A	2251	OMG	C6-N1	-2.40	1.34	1.37
1	1A	2605	PSU	C6-C5	2.40	1.38	1.35
54	1w	8	4SU	C2-N1	2.39	1.42	1.38
54	1w	8	4SU	C4-N3	-2.39	1.35	1.37
32	1a	1404	5MC	C6-N1	-2.39	1.34	1.38
1	2A	2552	OMU	C4-N3	-2.38	1.34	1.38
54	2w	54	5MU	C4-C5	2.37	1.48	1.44
1	1A	1939	5MU	C6-N1	-2.36	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	1x	54	5MU	C2-N1	2.36	1.42	1.38
1	1A	2503	2MA	C2-N3	2.36	1.36	1.31
1	2A	1939	5MU	C2-N3	-2.35	1.33	1.38
55	1x	55	PSU	C4-N3	-2.35	1.34	1.38
57	1y	55	PSU	C4-N3	-2.34	1.34	1.38
55	1x	32	5MC	C6-N1	-2.34	1.34	1.38
57	2y	55	PSU	C4-N3	-2.33	1.34	1.38
1	1A	1915	5MU	C4-C5	2.32	1.48	1.44
1	2A	1939	5MU	C4-C5	2.32	1.48	1.44
32	2a	1207	2MG	C6-N1	-2.31	1.34	1.37
1	1A	2552	OMU	C4-N3	-2.30	1.34	1.38
1	1A	1939	5MU	C2-N3	-2.30	1.33	1.38
54	1w	54	5MU	C4-N3	-2.29	1.34	1.38
54	1w	76	L3X	C5-N7	-2.29	1.31	1.39
32	1a	1207	2MG	C6-N1	-2.28	1.34	1.37
55	2x	54	5MU	C2-N1	2.28	1.42	1.38
55	1x	8	4SU	O2-C2	2.27	1.27	1.23
1	1A	1939	5MU	C2-N1	2.27	1.42	1.38
32	1a	1400	5MC	C6-N1	-2.25	1.34	1.38
32	1a	967	5MC	C6-N1	-2.25	1.34	1.38
1	2A	2552	OMU	C5-C4	2.25	1.48	1.43
57	1y	8	4SU	C5-C4	-2.23	1.39	1.42
1	1A	1962	5MC	C6-N1	-2.22	1.34	1.38
32	2a	1400	5MC	C6-N1	-2.21	1.34	1.38
57	2y	8	4SU	C2-N1	2.21	1.42	1.38
32	2a	1407	5MC	C6-N1	-2.19	1.34	1.38
57	1y	8	4SU	C2-N1	2.19	1.42	1.38
32	2a	967	5MC	C6-N1	-2.18	1.34	1.38
55	2x	76	8AN	C5-N7	-2.17	1.31	1.39
1	2A	1942	5MC	C6-N1	-2.16	1.34	1.38
1	2A	1915	5MU	C6-N1	-2.16	1.34	1.38
54	2w	8	4SU	C4-N3	-2.16	1.35	1.37
32	2a	1404	5MC	C6-N1	-2.15	1.34	1.38
54	2w	76	L3X	C5-N7	-2.15	1.31	1.39
55	1x	54	5MU	C4-C5	2.13	1.48	1.44
1	2A	1939	5MU	C6-N1	-2.13	1.34	1.38
57	1y	54	5MU	C6-N1	-2.13	1.34	1.38
57	1y	8	4SU	C2-N3	-2.11	1.34	1.38
57	2y	54	5MU	C2-N3	-2.10	1.34	1.38
55	2x	32	5MC	C6-N1	-2.09	1.34	1.38
55	1x	76	8AN	C5-N7	-2.09	1.32	1.39
55	2x	8	4SU	C6-C5	2.08	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1a	1498	UR3	C2-N1	2.06	1.41	1.38
1	1A	2552	OMU	C2-N3	-2.06	1.34	1.38
1	1A	2605	PSU	C2-N3	-2.06	1.34	1.37
55	1x	54	5MU	C6-N1	-2.06	1.34	1.38
1	1A	2552	OMU	C5-C4	2.05	1.48	1.43
1	1A	2503	2MA	C6-N1	-2.05	1.33	1.38
32	1a	1407	5MC	C6-N1	-2.03	1.34	1.38
57	2y	8	4SU	C2-N3	-2.03	1.34	1.38
55	2x	54	5MU	C2-N3	-2.01	1.34	1.38
55	1x	54	5MU	C2-N3	-2.01	1.34	1.38
1	2A	2552	OMU	C6-C5	2.01	1.39	1.35

All (231) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1l	92	0TD	CSB-SB-CB	-10.35	83.71	102.44
54	2w	8	4SU	C4-N3-C2	-8.52	119.06	127.34
43	2l	92	0TD	CSB-SB-CB	-7.25	89.32	102.44
54	2w	8	4SU	C5-C4-N3	7.12	121.30	114.69
1	2A	2605	PSU	N1-C2-N3	6.49	122.49	115.13
32	2a	516	PSU	N1-C2-N3	6.38	122.35	115.13
54	1w	8	4SU	C4-N3-C2	-6.27	121.25	127.34
1	2A	1917	PSU	N1-C2-N3	6.23	122.19	115.13
54	2w	8	4SU	C5-C4-S4	-6.13	116.57	124.47
55	2x	55	PSU	N1-C2-N3	6.09	122.03	115.13
1	2A	1939	5MU	C4-N3-C2	-6.04	119.53	127.35
32	1a	516	PSU	N1-C2-N3	6.02	121.95	115.13
55	1x	55	PSU	N1-C2-N3	5.98	121.91	115.13
54	2w	55	PSU	N1-C2-N3	5.94	121.86	115.13
57	1y	55	PSU	N1-C2-N3	5.91	121.82	115.13
54	1w	55	PSU	N1-C2-N3	5.89	121.80	115.13
57	2y	55	PSU	N1-C2-N3	5.83	121.73	115.13
54	1w	8	4SU	C5-C4-N3	5.82	120.09	114.69
1	1A	1911	PSU	N1-C2-N3	5.81	121.71	115.13
1	2A	1939	5MU	N3-C2-N1	5.80	122.58	114.89
1	1A	1917	PSU	N1-C2-N3	5.78	121.68	115.13
1	1A	2605	PSU	N1-C2-N3	5.78	121.68	115.13
1	2A	1911	PSU	N1-C2-N3	5.74	121.64	115.13
57	2y	8	4SU	C4-N3-C2	-5.68	121.82	127.34
32	2a	1498	UR3	C4-N3-C2	-5.66	119.23	124.56
32	1a	1498	UR3	C4-N3-C2	-5.63	119.26	124.56
54	2w	76	L3X	N3-C2-N1	-5.59	119.94	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	2x	76	8AN	N3-C2-N1	-5.56	119.99	128.68
54	1w	76	L3X	N3-C2-N1	-5.51	120.07	128.68
57	2y	8	4SU	C5-C4-N3	5.46	119.75	114.69
55	1x	76	8AN	N3-C2-N1	-5.25	120.47	128.68
1	2A	1915	5MU	C4-N3-C2	-5.23	120.58	127.35
57	1y	8	4SU	C5-C4-N3	5.11	119.43	114.69
1	1A	1915	5MU	N3-C2-N1	5.10	121.66	114.89
1	2A	1915	5MU	C5-C4-N3	5.08	119.64	115.31
1	2A	1939	5MU	C5-C4-N3	5.05	119.62	115.31
1	1A	2552	OMU	N3-C2-N1	4.95	121.46	114.89
1	1A	1939	5MU	C4-N3-C2	-4.94	120.96	127.35
1	2A	2552	OMU	N3-C2-N1	4.94	121.44	114.89
57	1y	54	5MU	C4-N3-C2	-4.92	120.99	127.35
1	1A	1915	5MU	C4-N3-C2	-4.90	121.01	127.35
1	2A	1939	5MU	C5-C6-N1	-4.84	118.36	123.34
55	1x	8	4SU	C6-C5-C4	-4.79	115.80	119.95
32	2a	1519	MA6	N3-C2-N1	-4.78	121.20	128.68
57	1y	54	5MU	N3-C2-N1	4.76	121.21	114.89
32	1a	1518	MA6	N3-C2-N1	-4.76	121.24	128.68
1	2A	2605	PSU	C4-N3-C2	-4.72	119.54	126.34
32	1a	1519	MA6	N3-C2-N1	-4.71	121.31	128.68
57	1y	8	4SU	C4-N3-C2	-4.70	122.77	127.34
1	1A	1939	5MU	C5-C6-N1	-4.70	118.50	123.34
54	1w	54	5MU	C4-N3-C2	-4.69	121.28	127.35
55	2x	54	5MU	N3-C2-N1	4.67	121.09	114.89
55	2x	54	5MU	C4-N3-C2	-4.65	121.33	127.35
54	1w	54	5MU	N3-C2-N1	4.64	121.05	114.89
1	1A	1939	5MU	C5-C4-N3	4.63	119.26	115.31
1	2A	1915	5MU	N3-C2-N1	4.61	121.01	114.89
1	2A	1915	5MU	O4-C4-C5	-4.58	119.59	124.90
1	1A	2552	OMU	C4-N3-C2	-4.53	120.61	126.58
1	1A	1939	5MU	N3-C2-N1	4.43	120.77	114.89
54	1w	8	4SU	C5-C4-S4	-4.37	118.84	124.47
55	1x	54	5MU	C4-N3-C2	-4.36	121.71	127.35
1	1A	2605	PSU	C4-N3-C2	-4.35	120.08	126.34
57	2y	54	5MU	C5-C4-N3	4.32	119.00	115.31
32	2a	1518	MA6	N3-C2-N1	-4.26	122.02	128.68
1	2A	2552	OMU	C4-N3-C2	-4.25	120.98	126.58
57	2y	54	5MU	N3-C2-N1	4.24	120.52	114.89
55	1x	54	5MU	N3-C2-N1	4.21	120.48	114.89
57	1y	54	5MU	C5-C4-N3	4.19	118.88	115.31
57	2y	54	5MU	C4-N3-C2	-4.18	121.94	127.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	1x	54	5MU	C5-C4-N3	4.18	118.88	115.31
1	1A	1915	5MU	C5-C4-N3	4.18	118.88	115.31
55	2x	54	5MU	C5-C4-N3	4.16	118.86	115.31
55	1x	55	PSU	C4-N3-C2	-4.09	120.44	126.34
32	2a	516	PSU	C4-N3-C2	-4.08	120.45	126.34
32	1a	516	PSU	C4-N3-C2	-4.06	120.49	126.34
54	1w	54	5MU	O4-C4-C5	-4.05	120.21	124.90
54	1w	54	5MU	C5-C4-N3	4.03	118.75	115.31
55	1x	8	4SU	S4-C4-N3	-4.01	116.25	120.21
1	2A	1939	5MU	O4-C4-C5	-4.01	120.26	124.90
1	1A	1917	PSU	C4-N3-C2	-4.01	120.57	126.34
1	2A	1917	PSU	C4-N3-C2	-4.00	120.58	126.34
55	1x	32	5MC	C5-C6-N1	-3.99	119.24	123.34
32	1a	967	5MC	C5-C6-N1	-3.97	119.26	123.34
32	2a	516	PSU	O2-C2-N1	-3.96	118.43	122.79
57	1y	55	PSU	O2-C2-N1	-3.95	118.44	122.79
55	1x	54	5MU	O4-C4-C5	-3.91	120.38	124.90
54	2w	8	4SU	N3-C2-N1	3.89	120.05	114.89
1	1A	1915	5MU	O4-C4-C5	-3.89	120.40	124.90
54	2w	55	PSU	C4-N3-C2	-3.88	120.75	126.34
57	1y	54	5MU	O4-C4-C5	-3.87	120.41	124.90
55	1x	8	4SU	O2-C2-N1	3.85	127.91	122.79
55	2x	54	5MU	O4-C4-C5	-3.85	120.44	124.90
1	1A	1911	PSU	C4-N3-C2	-3.84	120.81	126.34
32	2a	1400	5MC	C5-C6-N1	-3.83	119.39	123.34
55	2x	55	PSU	C4-N3-C2	-3.82	120.83	126.34
55	2x	8	4SU	C5-C4-N3	3.75	118.17	114.69
54	2w	54	5MU	C5-C4-N3	3.74	118.51	115.31
1	1A	1942	5MC	C5-C6-N1	-3.73	119.50	123.34
55	1x	8	4SU	C5-C4-N3	3.72	118.14	114.69
1	2A	1942	5MC	C5-C6-N1	-3.67	119.56	123.34
1	2A	1962	5MC	C5-C6-N1	-3.67	119.56	123.34
54	1w	55	PSU	C4-N3-C2	-3.65	121.08	126.34
57	2y	55	PSU	O2-C2-N1	-3.63	118.79	122.79
55	1x	54	5MU	C5-C6-N1	-3.63	119.60	123.34
57	2y	55	PSU	C4-N3-C2	-3.62	121.12	126.34
54	2w	55	PSU	O2-C2-N1	-3.62	118.80	122.79
54	2w	54	5MU	N3-C2-N1	3.60	119.66	114.89
57	1y	55	PSU	C4-N3-C2	-3.59	121.17	126.34
1	2A	1911	PSU	C4-N3-C2	-3.58	121.18	126.34
54	2w	54	5MU	C4-N3-C2	-3.57	122.73	127.35
55	2x	32	5MC	C5-C6-N1	-3.54	119.69	123.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2w	54	5MU	O4-C4-C5	-3.53	120.81	124.90
55	1x	55	PSU	O2-C2-N1	-3.53	118.91	122.79
57	2y	8	4SU	C5-C4-S4	-3.52	119.93	124.47
57	2y	8	4SU	N3-C2-N1	3.50	119.54	114.89
55	2x	55	PSU	O2-C2-N1	-3.50	118.93	122.79
57	1y	54	5MU	C5-C6-N1	-3.49	119.75	123.34
54	1w	55	PSU	O2-C2-N1	-3.48	118.96	122.79
1	1A	1917	PSU	O2-C2-N1	-3.46	118.98	122.79
1	2A	1939	5MU	O2-C2-N1	-3.44	118.21	122.79
1	2A	1915	5MU	C5-C6-N1	-3.44	119.80	123.34
1	1A	1962	5MC	C5-C6-N1	-3.42	119.82	123.34
32	2a	1404	5MC	C5-C6-N1	-3.39	119.85	123.34
54	1w	8	4SU	N3-C2-N1	3.39	119.39	114.89
32	1a	1407	5MC	C5-C6-N1	-3.39	119.86	123.34
32	2a	1519	MA6	C4-C5-N7	-3.38	105.88	109.40
57	2y	54	5MU	O4-C4-C5	-3.35	121.02	124.90
1	2A	1917	PSU	O2-C2-N1	-3.34	119.12	122.79
55	2x	54	5MU	C5-C6-N1	-3.29	119.95	123.34
55	1x	76	8AN	O4'-C1'-C2'	-3.29	102.12	106.93
32	2a	1407	5MC	C5-C6-N1	-3.28	119.96	123.34
32	1a	1400	5MC	C5-C6-N1	-3.28	119.96	123.34
32	1a	1404	5MC	C5-C6-N1	-3.21	120.03	123.34
1	2A	2552	OMU	O2-C2-N1	-3.21	118.52	122.79
32	1a	1519	MA6	C4-C5-N7	-3.21	106.06	109.40
32	2a	967	5MC	C5-C6-N1	-3.20	120.05	123.34
54	2w	8	4SU	O2-C2-N1	-3.18	118.55	122.79
1	2A	2605	PSU	O2-C2-N1	-3.07	119.41	122.79
1	1A	2605	PSU	O2-C2-N1	-3.05	119.44	122.79
1	2A	1911	PSU	O2-C2-N1	-3.03	119.46	122.79
55	2x	8	4SU	C1'-N1-C2	3.03	123.05	117.57
1	1A	2552	OMU	O4-C4-C5	-3.00	119.89	125.16
1	1A	1939	5MU	O4-C4-C5	-2.98	121.45	124.90
43	2l	92	0TD	OD2-CG-CB	2.95	119.52	113.15
55	1x	32	5MC	C5-C4-N3	-2.93	118.51	121.67
55	2x	76	8AN	O4'-C1'-C2'	-2.93	102.64	106.93
1	2A	2251	OMG	O6-C6-C5	-2.89	118.73	124.37
32	2a	1518	MA6	C4-C5-N7	-2.88	106.40	109.40
32	1a	516	PSU	O2-C2-N1	-2.88	119.62	122.79
1	2A	2552	OMU	C5-C4-N3	2.87	119.14	114.84
32	1a	1404	5MC	C5-C4-N3	-2.85	118.60	121.67
1	1A	1942	5MC	C5-C4-N3	-2.82	118.63	121.67
32	2a	1407	5MC	C5-C4-N3	-2.82	118.63	121.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2251	OMG	C5-C6-N1	2.82	118.93	113.95
57	1y	8	4SU	N3-C2-N1	2.80	118.61	114.89
57	2y	54	5MU	C5-C6-N1	-2.78	120.48	123.34
54	1w	54	5MU	C5-C6-N1	-2.76	120.50	123.34
1	1A	1911	PSU	O2-C2-N1	-2.74	119.77	122.79
1	1A	2552	OMU	C5-C4-N3	2.73	118.93	114.84
32	1a	1400	5MC	C5-C4-N3	-2.72	118.74	121.67
43	1l	92	0TD	OD2-CG-CB	2.72	119.03	113.15
54	1w	8	4SU	C1'-N1-C2	2.71	122.47	117.57
1	1A	1915	5MU	C5-C6-N1	-2.69	120.57	123.34
32	2a	1404	5MC	C5-C4-N3	-2.68	118.79	121.67
32	1a	1518	MA6	C4-C5-N7	-2.66	106.63	109.40
57	1y	8	4SU	C5-C4-S4	-2.65	121.05	124.47
1	1A	2552	OMU	O2-C2-N1	-2.65	119.26	122.79
1	1A	1920	OMC	O2-C2-N3	-2.64	118.03	122.33
1	1A	1962	5MC	C5-C4-N3	-2.63	118.84	121.67
55	2x	32	5MC	O2-C2-N3	-2.62	118.07	122.33
1	2A	2605	PSU	C5-C6-N1	-2.58	118.24	122.11
1	1A	2503	2MA	C5-C6-N1	2.55	118.43	114.02
1	2A	2552	OMU	O4-C4-C5	-2.55	120.68	125.16
55	2x	8	4SU	C6-C5-C4	-2.54	117.75	119.95
1	2A	1962	5MC	C5-C4-N3	-2.53	118.94	121.67
32	1a	1407	5MC	C5-C4-N3	-2.53	118.95	121.67
32	1a	1207	2MG	C8-N7-C5	2.52	107.79	102.99
32	2a	1407	5MC	O2-C2-N3	-2.51	118.26	122.33
55	2x	32	5MC	C5-C4-N3	-2.49	118.99	121.67
32	1a	967	5MC	C5-C4-N3	-2.48	119.00	121.67
1	2A	1942	5MC	C5-C4-N3	-2.46	119.02	121.67
32	2a	966	M2G	C8-N7-C5	2.42	107.61	102.99
32	1a	1402	4OC	C6-C5-C4	2.41	119.91	116.96
1	2A	2503	2MA	C5-C6-N1	2.39	118.14	114.02
56	2z	1	FME	C-CA-N	2.39	114.04	109.73
32	2a	1207	2MG	C8-N7-C5	2.39	107.54	102.99
1	1A	2251	OMG	C5-C6-N1	2.38	118.16	113.95
57	2y	8	4SU	C1'-N1-C2	2.36	121.85	117.57
32	2a	966	M2G	C5-C6-N1	2.36	118.12	113.95
54	2w	54	5MU	C5-C6-N1	-2.36	120.92	123.34
1	1A	2251	OMG	C8-N7-C5	2.31	107.40	102.99
32	2a	1400	5MC	C5-C4-N3	-2.31	119.18	121.67
54	1w	55	PSU	C6-C5-C4	-2.31	116.58	118.20
32	2a	1402	4OC	C6-C5-C4	2.30	119.78	116.96
55	1x	8	4SU	C1'-N1-C2	2.27	121.67	117.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	1y	54	5MU	O2-C2-N1	-2.27	119.78	122.79
32	1a	966	M2G	C8-N7-C5	2.26	107.31	102.99
1	1A	2503	2MA	C8-N7-C5	2.25	107.28	102.99
57	2y	54	5MU	C1'-N1-C2	2.23	121.62	117.57
54	2w	8	4SU	C1'-N1-C2	2.23	121.60	117.57
32	1a	1404	5MC	O2-C2-N3	-2.23	118.71	122.33
32	2a	1404	5MC	O2-C2-N3	-2.22	118.72	122.33
54	1w	54	5MU	O2-C2-N1	-2.22	119.84	122.79
54	2w	54	5MU	C5M-C5-C4	2.21	121.20	118.77
32	2a	1207	2MG	C5-C6-N1	2.19	117.82	113.95
55	1x	55	PSU	C5-C6-N1	-2.18	118.84	122.11
1	1A	1942	5MC	CM5-C5-C6	-2.17	119.95	122.85
1	1A	1962	5MC	O2-C2-N3	-2.17	118.80	122.33
1	2A	1920	OMC	O2-C2-N3	-2.17	118.80	122.33
32	1a	966	M2G	C5-C6-N1	2.15	117.75	113.95
1	2A	1917	PSU	C5-C6-N1	-2.14	118.89	122.11
32	2a	516	PSU	C5-C6-N1	-2.13	118.91	122.11
32	2a	516	PSU	O4'-C1'-C2'	2.13	108.15	105.14
1	2A	2503	2MA	C8-N7-C5	2.13	107.05	102.99
32	2a	967	5MC	C1'-N1-C6	-2.11	117.62	121.12
1	1A	2552	OMU	C2'-C1'-N1	-2.10	110.14	114.22
1	1A	2251	OMG	O6-C6-C5	-2.10	120.27	124.37
1	2A	2251	OMG	C8-N7-C5	2.10	106.99	102.99
32	2a	967	5MC	C5-C4-N3	-2.09	119.42	121.67
57	2y	54	5MU	O2-C2-N3	-2.09	117.61	121.50
1	1A	1911	PSU	O4'-C1'-C2'	2.09	108.09	105.14
32	1a	1400	5MC	O2-C2-N3	-2.08	118.95	122.33
55	1x	8	4SU	O2-C2-N3	-2.07	117.64	121.50
32	2a	1402	4OC	CM4-N4-C4	-2.03	118.49	122.45
32	2a	1400	5MC	O2-C2-N3	-2.03	119.04	122.33
1	1A	1915	5MU	O2-C2-N1	-2.02	120.11	122.79
55	2x	8	4SU	O2-C2-N3	-2.01	117.75	121.50
1	1A	1915	5MU	C5M-C5-C4	2.01	120.98	118.77
32	2a	1498	UR3	C3U-N3-C4	2.01	120.76	117.89
32	1a	516	PSU	O4'-C1'-C2'	2.01	107.97	105.14
54	1w	54	5MU	C5M-C5-C4	2.00	120.97	118.77

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	1207	2MG	N3-C2-N2-CM2

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Mol	Chain	Res	Type	Atoms
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1207	2MG	N3-C2-N2-CM2
54	2w	76	L3X	C3'-C4'-C5'-O5'
54	2w	76	L3X	O4'-C4'-C5'-O5'
55	1x	76	8AN	C3'-C4'-C5'-O5'
55	2x	76	8AN	C3'-C4'-C5'-O5'
57	2y	55	PSU	C3'-C4'-C5'-O5'
57	2y	55	PSU	O4'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
57	2y	8	4SU	O4'-C4'-C5'-O5'
32	2a	1402	4OC	O4'-C4'-C5'-O5'
55	1x	76	8AN	O4'-C4'-C5'-O5'
55	2x	76	8AN	O4'-C4'-C5'-O5'
57	2y	8	4SU	C3'-C4'-C5'-O5'
57	2y	54	5MU	O4'-C4'-C5'-O5'
56	1z	1	FME	N-CA-CB-CG
32	1a	967	5MC	O4'-C4'-C5'-O5'
32	2a	527	G7M	C3'-C4'-C5'-O5'
32	2a	1402	4OC	C3'-C4'-C5'-O5'
57	2y	54	5MU	C3'-C4'-C5'-O5'
32	2a	1519	MA6	O4'-C4'-C5'-O5'
56	1z	1	FME	CB-CG-SD-CE
32	2a	527	G7M	O4'-C4'-C5'-O5'
43	1l	92	0TD	CG-CB-SB-CSB
43	2l	92	0TD	CG-CB-SB-CSB
55	1x	76	8AN	C4'-C5'-O5'-P
32	1a	527	G7M	C3'-C4'-C5'-O5'
32	1a	1402	4OC	O4'-C4'-C5'-O5'
32	1a	1519	MA6	C4'-C5'-O5'-P
55	2x	76	8AN	C4'-C5'-O5'-P
56	1z	1	FME	C-CA-CB-CG
1	1A	2503	2MA	C4'-C5'-O5'-P
32	1a	527	G7M	C4'-C5'-O5'-P
1	2A	2503	2MA	O4'-C4'-C5'-O5'
57	1y	55	PSU	O4'-C1'-C5-C4
57	2y	55	PSU	O4'-C1'-C5-C4
1	1A	2503	2MA	O4'-C4'-C5'-O5'
43	2l	92	0TD	SB-CB-CG-OD2
32	1a	967	5MC	C3'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
1	1A	1920	OMC	C2'-C1'-N1-C2
55	2x	8	4SU	C2'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
57	1y	55	PSU	O4'-C1'-C5-C6
57	2y	54	5MU	C2'-C1'-N1-C2
32	2a	1519	MA6	C4'-C5'-O5'-P
1	1A	1962	5MC	C2'-C1'-N1-C6

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 2669 ligands modelled in this entry, 2665 are monoatomic - leaving 4 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	$\# Z > 2$
62	SF4	2d	303	35	0,12,12	-	-	-		
62	SF4	1d	302	35	0,12,12	-	-	-		
60	CLM	2w	103	-	19,20,20	0.84	0	23,27,27	0.87	1 (4%)
60	CLM	1A	4087	-	19,20,20	0.97	1 (5%)	23,27,27	1.30	3 (13%)

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
62	SF4	2d	303	35	-	-	0/6/5/5
62	SF4	1d	302	35	-	-	0/6/5/5
60	CLM	2w	103	-	-	2/20/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	CLM	1A	4087	-	-	4/20/22/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	1A	4087	CLM	C6-C5	-2.22	1.48	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	1A	4087	CLM	C8-C9-N9	3.09	121.70	119.38
60	1A	4087	CLM	C6-C5-C3	3.06	117.02	111.64
60	1A	4087	CLM	O5-C5-C6	-2.89	104.90	111.19
60	2w	103	CLM	C8-C9-N9	2.11	120.97	119.38

There are no chirality outliers.

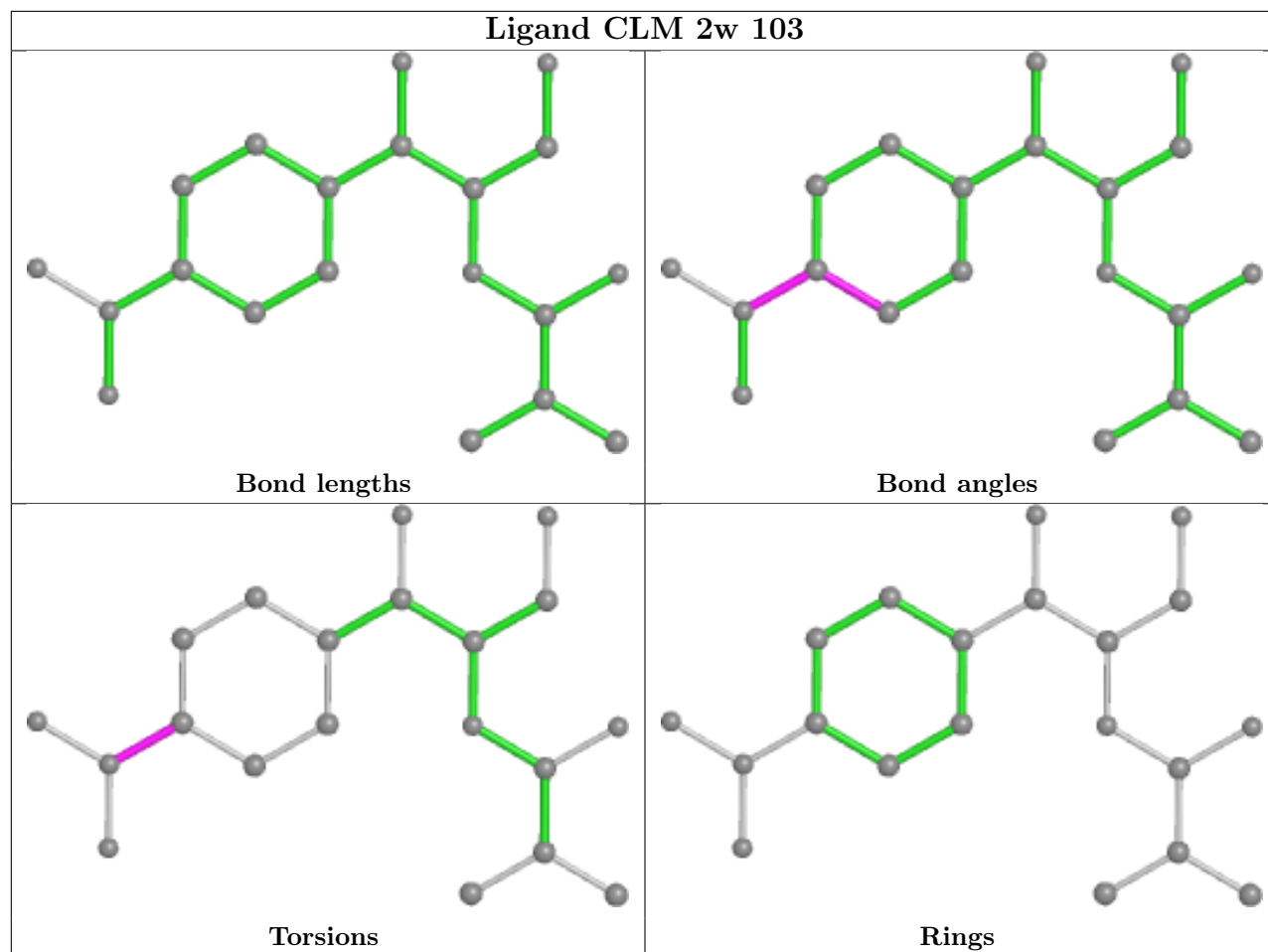
All (6) torsion outliers are listed below:

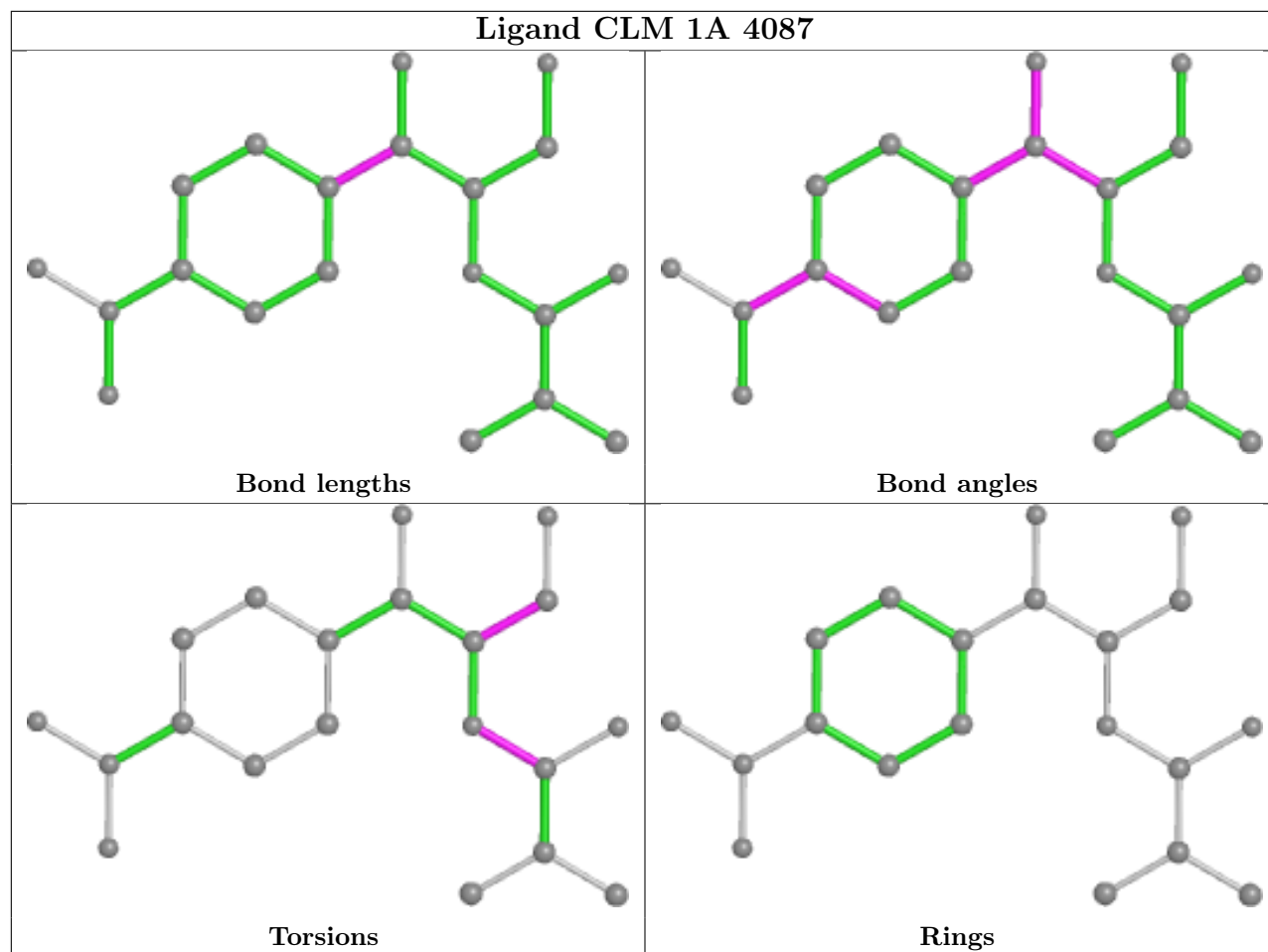
Mol	Chain	Res	Type	Atoms
60	1A	4087	CLM	N2-C3-C4-O4
60	1A	4087	CLM	C5-C3-C4-O4
60	2w	103	CLM	C8-C9-N9-O9B
60	2w	103	CLM	C10-C9-N9-O9B
60	1A	4087	CLM	O2-C2-N2-C3
60	1A	4087	CLM	C1-C2-N2-C3

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1A	2860/2915 (98%)	0.38	132 (4%) 32 39	28, 45, 105, 116	0
1	2A	2789/2915 (95%)	0.20	111 (3%) 38 45	42, 67, 102, 116	0
2	1B	120/121 (99%)	-0.22	0 100 100	38, 60, 73, 98	0
2	2B	120/121 (99%)	-0.31	0 100 100	70, 87, 94, 103	0
3	1D	275/276 (99%)	0.69	3 (1%) 80 85	28, 46, 59, 88	0
3	2D	275/276 (99%)	0.89	6 (2%) 62 68	41, 59, 72, 88	0
4	1E	204/206 (99%)	0.54	1 (0%) 91 94	28, 49, 66, 82	0
4	2E	204/206 (99%)	0.55	9 (4%) 34 41	46, 69, 81, 90	0
5	1F	202/210 (96%)	0.50	1 (0%) 91 94	26, 51, 73, 94	0
5	2F	202/210 (96%)	0.70	14 (6%) 16 20	46, 77, 88, 94	0
6	1G	181/182 (99%)	0.51	9 (4%) 28 34	52, 69, 83, 96	0
6	2G	181/182 (99%)	1.43	49 (27%) 0 0	76, 88, 94, 99	0
7	1H	174/180 (96%)	0.32	3 (1%) 70 76	47, 61, 74, 83	0
7	2H	174/180 (96%)	2.25	84 (48%) 0 0	79, 92, 100, 102	0
8	1I	146/148 (98%)	0.62	9 (6%) 20 24	53, 81, 89, 92	0
8	2I	146/148 (98%)	0.59	12 (8%) 11 14	64, 82, 89, 94	0
9	1N	140/140 (100%)	0.50	1 (0%) 87 90	33, 45, 66, 81	0
9	2N	140/140 (100%)	0.50	5 (3%) 42 49	61, 76, 87, 96	0
10	1O	122/122 (100%)	0.64	0 100 100	38, 49, 66, 71	0
10	2O	122/122 (100%)	0.61	4 (3%) 46 53	58, 68, 79, 84	0
11	1P	149/150 (99%)	0.48	1 (0%) 87 90	29, 53, 74, 84	0
11	2P	149/150 (99%)	1.24	31 (20%) 1 0	51, 76, 91, 96	0
12	1Q	141/141 (100%)	0.58	0 100 100	32, 50, 64, 85	0
12	2Q	141/141 (100%)	1.09	26 (18%) 1 1	63, 76, 86, 93	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	0.37	0 100 100	32, 44, 58, 65	0
13	2R	118/118 (100%)	0.54	1 (0%) 86 89	48, 63, 74, 80	0
14	1S	110/112 (98%)	0.30	1 (0%) 84 88	45, 59, 72, 75	0
14	2S	110/112 (98%)	1.22	27 (24%) 0 0	70, 82, 89, 94	0
15	1T	131/146 (89%)	0.29	0 100 100	41, 54, 76, 84	0
15	2T	131/146 (89%)	0.54	7 (5%) 26 31	63, 71, 84, 91	0
16	1U	116/118 (98%)	0.51	2 (1%) 70 76	30, 39, 55, 69	0
16	2U	116/118 (98%)	0.58	5 (4%) 35 42	55, 74, 86, 94	0
17	1V	101/101 (100%)	0.39	1 (0%) 82 86	31, 48, 64, 78	0
17	2V	101/101 (100%)	0.70	10 (9%) 7 9	51, 82, 89, 92	0
18	1W	112/113 (99%)	0.49	1 (0%) 84 88	31, 40, 58, 90	0
18	2W	112/113 (99%)	0.68	3 (2%) 54 61	50, 60, 75, 95	0
19	1X	95/96 (98%)	0.54	2 (2%) 63 70	35, 47, 72, 85	0
19	2X	95/96 (98%)	0.54	4 (4%) 36 42	52, 68, 80, 96	0
20	1Y	107/110 (97%)	0.45	2 (1%) 66 73	45, 59, 73, 88	0
20	2Y	107/110 (97%)	0.87	12 (11%) 5 7	66, 81, 89, 95	0
21	1Z	154/206 (74%)	0.69	19 (12%) 4 5	46, 70, 93, 99	0
21	2Z	160/206 (77%)	2.12	75 (46%) 0 0	79, 89, 99, 101	0
22	10	83/85 (97%)	0.60	1 (1%) 79 84	33, 46, 65, 78	0
22	20	83/85 (97%)	0.74	4 (4%) 30 37	56, 73, 85, 88	0
23	11	97/98 (98%)	0.78	6 (6%) 20 24	36, 54, 76, 87	0
23	21	97/98 (98%)	0.54	2 (2%) 63 70	46, 64, 81, 85	0
24	12	70/72 (97%)	0.46	0 100 100	43, 58, 69, 78	0
24	22	70/72 (97%)	0.71	6 (8%) 10 12	66, 79, 86, 88	0
25	13	59/60 (98%)	0.39	0 100 100	34, 43, 70, 89	0
25	23	59/60 (98%)	1.00	12 (20%) 1 1	66, 76, 86, 92	0
26	14	69/71 (97%)	1.02	15 (21%) 0 0	65, 83, 96, 99	0
26	24	69/71 (97%)	2.30	36 (52%) 0 0	87, 95, 101, 101	0
27	15	59/60 (98%)	0.47	1 (1%) 70 76	28, 42, 64, 69	0
27	25	59/60 (98%)	0.62	2 (3%) 45 52	46, 62, 80, 89	0
28	16	53/54 (98%)	0.37	0 100 100	41, 51, 65, 70	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.52	1 (1%) 66 73	60, 71, 78, 85	0
29	17	48/49 (97%)	0.85	5 (10%) 6 8	29, 36, 70, 76	0
29	27	48/49 (97%)	1.06	5 (10%) 6 8	43, 50, 74, 81	0
30	18	64/65 (98%)	0.46	0 100 100	34, 42, 50, 63	0
30	28	64/65 (98%)	0.68	2 (3%) 49 56	55, 65, 73, 80	0
31	19	37/37 (100%)	0.75	1 (2%) 54 61	39, 48, 66, 69	0
31	29	37/37 (100%)	1.91	16 (43%) 0 0	72, 79, 89, 92	0
32	1a	1488/1521 (97%)	0.09	57 (3%) 40 47	44, 79, 103, 117	0
32	2a	1491/1521 (98%)	0.14	71 (4%) 30 37	57, 85, 105, 115	0
33	1b	231/256 (90%)	0.90	36 (15%) 2 2	75, 87, 97, 105	0
33	2b	231/256 (90%)	1.80	92 (39%) 0 0	81, 93, 98, 100	0
34	1c	206/239 (86%)	1.33	52 (25%) 0 0	75, 85, 94, 99	0
34	2c	206/239 (86%)	1.88	93 (45%) 0 0	85, 92, 98, 103	0
35	1d	208/209 (99%)	0.92	28 (13%) 3 4	67, 82, 90, 98	0
35	2d	208/209 (99%)	1.12	41 (19%) 1 1	68, 77, 85, 90	0
36	1e	148/162 (91%)	0.60	7 (4%) 31 38	55, 75, 84, 89	0
36	2e	148/162 (91%)	1.43	39 (26%) 0 0	72, 85, 92, 98	0
37	1f	100/101 (99%)	0.71	8 (8%) 12 15	65, 78, 85, 88	0
37	2f	100/101 (99%)	0.49	4 (4%) 38 45	71, 81, 88, 95	0
38	1g	155/156 (99%)	1.08	29 (18%) 1 1	73, 83, 94, 100	0
38	2g	155/156 (99%)	1.72	56 (36%) 0 0	79, 88, 97, 102	0
39	1h	137/138 (99%)	0.33	5 (3%) 42 49	64, 76, 82, 89	0
39	2h	137/138 (99%)	1.03	18 (13%) 3 4	78, 85, 90, 93	0
40	1i	127/128 (99%)	1.87	53 (41%) 0 0	69, 88, 93, 96	0
40	2i	127/128 (99%)	3.16	92 (72%) 0 0	78, 93, 98, 99	0
41	1j	97/105 (92%)	2.26	51 (52%) 0 0	73, 90, 96, 99	0
41	2j	96/105 (91%)	3.14	68 (70%) 0 0	86, 95, 100, 103	0
42	1k	114/129 (88%)	0.71	8 (7%) 16 19	50, 75, 88, 95	0
42	2k	114/129 (88%)	0.78	12 (10%) 6 8	65, 82, 91, 93	0
43	1l	121/132 (91%)	0.56	2 (1%) 70 76	55, 70, 79, 83	0
43	2l	121/132 (91%)	0.89	14 (11%) 4 6	69, 81, 88, 90	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	123/126 (97%)	0.88	12 (9%) 7 9	69, 82, 90, 98	0
44	2m	122/126 (96%)	2.15	47 (38%) 0 0	83, 91, 97, 101	0
45	1n	60/61 (98%)	1.54	17 (28%) 0 0	74, 83, 89, 91	0
45	2n	60/61 (98%)	3.90	49 (81%) 0 0	88, 94, 98, 100	0
46	1o	88/89 (98%)	0.27	4 (4%) 33 40	56, 72, 82, 89	0
46	2o	88/89 (98%)	0.63	4 (4%) 33 40	69, 82, 89, 94	0
47	1p	82/88 (93%)	1.41	20 (24%) 0 0	68, 81, 89, 96	0
47	2p	82/88 (93%)	0.79	6 (7%) 15 18	67, 76, 84, 88	0
48	1q	99/105 (94%)	0.62	4 (4%) 38 45	63, 74, 85, 86	0
48	2q	99/105 (94%)	0.91	12 (12%) 4 5	71, 81, 89, 94	0
49	1r	68/88 (77%)	0.56	4 (5%) 22 26	66, 75, 86, 89	0
49	2r	68/88 (77%)	0.71	2 (2%) 51 59	75, 81, 89, 90	0
50	1s	83/93 (89%)	1.67	34 (40%) 0 0	74, 85, 92, 96	0
50	2s	83/93 (89%)	2.80	52 (62%) 0 0	87, 95, 100, 104	0
51	1t	96/106 (90%)	1.03	22 (22%) 0 0	68, 80, 89, 91	0
51	2t	96/106 (90%)	0.83	10 (10%) 6 8	65, 79, 89, 90	0
52	1u	23/27 (85%)	2.14	13 (56%) 0 0	74, 80, 83, 85	0
52	2u	23/27 (85%)	2.49	14 (60%) 0 0	84, 90, 94, 96	0
53	1v	13/24 (54%)	1.83	5 (38%) 0 0	58, 82, 104, 108	0
53	2v	13/24 (54%)	1.72	5 (38%) 0 0	81, 93, 107, 113	0
54	1w	69/74 (93%)	3.38	50 (72%) 0 0	62, 106, 112, 114	0
54	2w	68/74 (91%)	3.44	43 (63%) 0 0	78, 108, 113, 115	0
55	1x	72/77 (93%)	-0.04	0 100 100	43, 76, 93, 96	0
55	2x	72/77 (93%)	-0.12	2 (2%) 53 60	62, 91, 99, 109	0
56	1z	2/3 (66%)	0.89	0 100 100	44, 44, 44, 46	0
56	2z	2/3 (66%)	1.37	0 100 100	64, 64, 64, 69	0
57	1y	70/74 (94%)	4.87	64 (91%) 0 0	68, 110, 113, 115	0
57	2y	70/74 (94%)	5.53	69 (98%) 0 0	80, 111, 115, 116	0
All	All	20889/21746 (96%)	0.69	2298 (11%) 5 7	26, 74, 99, 117	0

All (2298) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
54	2w	71	G	20.9
44	2m	123	ALA	20.6
44	2m	124	PRO	18.1
57	2y	36	C	14.1
57	1y	36	C	12.6
54	1w	70	C	12.3
57	1y	24	A	11.4
45	2n	34	TYR	11.4
57	1y	35	C	11.2
38	2g	154	TYR	11.0
44	1m	123	ALA	10.9
57	1y	34	C	10.7
54	2w	70	C	10.7
38	2g	156	TRP	10.6
57	2y	35	C	10.6
41	2j	47	PHE	10.4
44	1m	124	PRO	10.4
1	1A	2145	C	10.3
45	2n	39	LEU	10.3
57	2y	39	G	10.2
21	1Z	1	MET	10.1
54	1w	71	G	10.1
57	2y	37	A	9.9
34	2c	8	ILE	9.9
57	2y	34	C	9.8
54	2w	2	C	9.7
54	2w	72	C	9.7
21	2Z	144	LEU	9.5
54	2w	4	G	9.5
45	2n	38	GLY	9.5
57	2y	33	U	9.5
41	2j	20	ALA	9.5
1	2A	2145	C	9.4
57	1y	32	U	9.4
54	2w	3	G	9.4
44	2m	121	LYS	9.3
38	2g	80	VAL	9.2
54	2w	1	G	9.1
1	2A	2160	G	9.0
57	2y	23	A	8.9
40	1i	19	LEU	8.9
54	1w	4	G	8.8
54	1w	72	C	8.7

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Mol	Chain	Res	Type	RSRZ
1	2A	2146	C	8.7
1	1A	2115	G	8.6
1	2A	2159	G	8.6
57	2y	32	U	8.5
32	2a	1030(B)	C	8.5
1	2A	2138	C	8.5
57	2y	24	A	8.5
41	2j	63	PHE	8.3
57	2y	3	G	8.2
45	2n	35	ARG	8.2
57	1y	38	A	8.2
57	2y	26	G	8.2
45	2n	25	VAL	8.1
57	2y	29	A	8.0
32	1a	1036	G	8.0
34	2c	186	PHE	7.9
21	2Z	149	SER	7.7
40	2i	30	GLY	7.6
1	2A	2111	C	7.6
1	2A	2147	G	7.6
57	2y	28	G	7.6
41	2j	6	ILE	7.6
57	2y	1	G	7.5
57	2y	38	A	7.5
57	1y	39	G	7.4
57	2y	25	C	7.3
44	2m	122	LYS	7.3
32	1a	1003	G	7.2
57	2y	72	C	7.2
21	2Z	141	VAL	7.2
40	2i	14	VAL	7.2
40	2i	36	TYR	7.2
1	1A	2112	G	7.2
1	2A	2139	C	7.1
40	2i	19	LEU	7.0
54	1w	19	U	7.0
45	2n	2	ALA	7.0
1	1A	1059	G	7.0
1	1A	1096	A	7.0
54	1w	69	C	7.0
57	1y	13	C	7.0
57	2y	74	C	7.0

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Mol	Chain	Res	Type	RSRZ
33	2b	165	VAL	7.0
1	2A	2115	G	7.0
1	2A	2113	U	7.0
1	2A	2179	C	7.0
45	2n	37	PHE	7.0
33	2b	161	ALA	7.0
1	2A	2135	A	7.0
38	2g	81	GLY	7.0
44	2m	7	VAL	6.9
57	1y	23	A	6.9
26	24	49	PHE	6.9
7	2H	52	VAL	6.9
1	1A	2159	G	6.8
41	2j	65	LEU	6.8
32	2a	1036	G	6.8
50	2s	71	LEU	6.8
1	2A	2133	G	6.8
1	1A	1064	C	6.8
44	2m	102	ARG	6.7
41	2j	72	VAL	6.7
32	2a	1034	G	6.7
1	1A	2114	A	6.7
26	24	32	TYR	6.6
1	2A	2128	C	6.6
40	2i	66	ARG	6.6
7	2H	35	VAL	6.6
34	2c	184	TYR	6.6
45	2n	11	LYS	6.6
41	2j	10	GLY	6.6
54	2w	10	G	6.6
45	2n	42	ILE	6.5
53	1v	13	A	6.5
1	1A	1065	U	6.5
57	1y	33	U	6.5
1	2A	2134	A	6.4
1	2A	2129	C	6.4
1	1A	2117	A	6.4
1	2A	2155	G	6.4
40	2i	37	PHE	6.4
57	1y	56	C	6.4
54	1w	49	G	6.4
1	2A	2117	A	6.4

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Mol	Chain	Res	Type	RSRZ
1	2A	2112	G	6.4
21	1Z	149	SER	6.4
26	24	63	TYR	6.3
57	1y	31	C	6.3
57	2y	53	G	6.3
57	2y	31	C	6.3
57	1y	53	G	6.3
50	2s	38	SER	6.3
40	2i	102	LEU	6.3
31	29	37	GLY	6.3
50	1s	71	LEU	6.2
54	1w	3	G	6.2
1	2A	2802	G	6.2
57	2y	51	G	6.2
6	2G	139	LEU	6.2
57	1y	12	U	6.2
1	1A	2169	A	6.2
57	1y	21	A	6.2
38	1g	79	ARG	6.2
34	1c	184	TYR	6.2
1	1A	2174	C	6.2
41	1j	71	LEU	6.2
20	2Y	1	MET	6.2
45	2n	58	LYS	6.2
57	1y	30	G	6.1
38	1g	80	VAL	6.1
1	1A	1095	A	6.1
32	1a	1257	U	6.1
1	2A	2116	G	6.1
41	2j	66	ARG	6.1
57	2y	15	A	6.1
1	1A	2160	G	6.1
1	2A	2104	G	6.1
40	2i	82	ALA	6.1
40	1i	14	VAL	6.0
1	1A	2130	U	6.0
6	2G	152	LEU	6.0
57	2y	21	A	6.0
12	2Q	33	GLY	6.0
32	1a	1001(A)	G	6.0
57	1y	49	G	6.0
45	2n	36	PHE	6.0

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Mol	Chain	Res	Type	RSRZ
1	1A	1068	G	6.0
1	1A	2110	G	6.0
34	2c	182	ILE	6.0
50	2s	45	VAL	6.0
1	1A	2180	U	6.0
41	2j	85	LEU	6.0
1	1A	1098	A	6.0
1	1A	2146	C	6.0
1	2A	652(B)	A	6.0
6	2G	146	TYR	6.0
41	1j	98	ILE	6.0
41	1j	36	GLY	6.0
1	1A	2147	G	5.9
57	1y	1	G	5.9
33	2b	214	ILE	5.9
57	1y	22	G	5.9
32	2a	1033	G	5.9
33	1b	227	GLY	5.9
40	2i	27	THR	5.9
52	1u	18	TYR	5.9
57	2y	2	C	5.9
1	2A	2127	G	5.9
32	2a	1030(A)	G	5.9
7	2H	24	VAL	5.8
7	2H	37	VAL	5.8
41	1j	47	PHE	5.8
41	2j	40	LEU	5.8
1	2A	2110	G	5.8
26	24	67	TYR	5.8
53	1v	12	A	5.8
57	1y	37	A	5.8
36	2e	31	LEU	5.8
54	2w	49	G	5.8
57	2y	52	G	5.8
40	2i	15	ALA	5.8
1	2A	2131	G	5.8
50	2s	50	ALA	5.8
33	2b	228	GLY	5.8
40	1i	106	ALA	5.8
50	2s	80	TYR	5.8
57	2y	57	G	5.7
54	1w	10	G	5.7

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Mol	Chain	Res	Type	RSRZ
21	2Z	96	VAL	5.7
1	1A	1094	U	5.7
41	2j	71	LEU	5.7
32	1a	1030(B)	C	5.7
21	2Z	174	VAL	5.7
57	2y	73	U	5.7
57	2y	18	G	5.7
57	2y	19	U	5.7
57	2y	22	G	5.7
1	1A	2111	C	5.6
57	1y	48	C	5.6
33	2b	207	ALA	5.6
45	1n	2	ALA	5.6
7	2H	113	VAL	5.6
38	2g	16	LEU	5.6
1	1A	2131	G	5.6
40	1i	4	TYR	5.6
1	1A	2170	A	5.6
57	1y	25	C	5.6
1	2A	2168	G	5.6
32	1a	1002	G	5.6
48	1q	98	LEU	5.6
1	1A	2129	C	5.6
54	2w	13	C	5.6
57	2y	56	C	5.6
57	2y	43	U	5.6
1	2A	2154	G	5.6
57	1y	51	G	5.6
57	2y	42	C	5.6
41	1j	8	LEU	5.5
34	2c	7	PRO	5.5
1	2A	2114	A	5.5
1	1A	2141	G	5.5
57	1y	71	G	5.5
38	1g	156	TRP	5.5
21	2Z	139	VAL	5.5
40	2i	9	ARG	5.5
1	1A	1057	A	5.5
57	2y	14	A	5.5
50	1s	15	LEU	5.5
32	1a	1027	C	5.5
6	1G	146	TYR	5.5

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Mol	Chain	Res	Type	RSRZ
26	24	51	ASP	5.5
53	2v	12	A	5.5
1	1A	2116	G	5.5
1	1A	2120	G	5.5
21	2Z	57	ILE	5.4
38	2g	82	GLY	5.4
1	1A	2175	C	5.4
54	2w	31	C	5.4
50	2s	52	TYR	5.4
57	2y	30	G	5.4
57	2y	66	C	5.4
1	1A	2181	G	5.4
41	2j	74	ILE	5.4
57	2y	62	C	5.4
1	1A	2113	U	5.4
1	1A	1099	G	5.4
50	2s	12	ASP	5.4
23	11	2	SER	5.3
1	2A	2167	U	5.3
57	2y	65	U	5.3
32	1a	1026	G	5.3
40	2i	17	VAL	5.3
26	14	66	SER	5.3
1	2A	2130	U	5.3
1	2A	2123	G	5.3
50	2s	67	VAL	5.3
40	2i	5	TYR	5.3
50	2s	14	HIS	5.3
40	1i	15	ALA	5.3
34	1c	87	LEU	5.3
40	2i	7	THR	5.3
54	1w	50	A	5.3
57	1y	57	G	5.3
21	2Z	121	HIS	5.2
29	17	46	VAL	5.2
54	1w	61	C	5.2
40	2i	103	THR	5.2
1	1A	2177	C	5.2
1	1A	2179	C	5.2
7	2H	72	ILE	5.2
40	2i	8	GLY	5.2
7	2H	76	VAL	5.2

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Mol	Chain	Res	Type	RSRZ
40	2i	108	VAL	5.2
7	2H	157	TYR	5.2
33	2b	187	LEU	5.2
38	2g	27	ILE	5.2
57	2y	41	U	5.2
40	2i	33	PHE	5.2
44	2m	120	LYS	5.2
1	2A	2174	C	5.2
40	2i	10	ARG	5.2
7	2H	105	LEU	5.2
41	2j	27	ALA	5.1
29	27	48	LYS	5.1
57	1y	64	U	5.1
1	2A	229	A	5.1
57	1y	50	A	5.1
41	1j	38	ILE	5.1
1	1A	1060	U	5.1
38	2g	40	ALA	5.1
32	1a	1005	A	5.1
6	2G	140	ILE	5.1
32	2a	1257	U	5.1
57	1y	3	G	5.1
57	1y	5	G	5.1
41	2j	11	PHE	5.1
53	2v	24	A	5.1
57	2y	75	C	5.1
7	2H	48	GLY	5.1
1	1A	1081	U	5.1
54	2w	5	G	5.1
7	2H	96	ALA	5.1
52	2u	16	GLY	5.1
33	2b	211	ILE	5.1
57	1y	52	G	5.0
44	1m	2	ALA	5.0
45	2n	56	VAL	5.0
41	1j	4	ILE	5.0
50	2s	40	ILE	5.0
33	1b	232	PRO	5.0
45	2n	61	TRP	5.0
1	2A	2182	G	5.0
54	1w	59	U	5.0
41	2j	8	LEU	5.0

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Mol	Chain	Res	Type	RSRZ
38	2g	32	ARG	5.0
3	1D	276	LYS	5.0
25	23	26	LEU	5.0
6	2G	142	PRO	5.0
26	24	52	THR	5.0
32	1a	1038	C	5.0
32	1a	1035	A	5.0
24	22	1	MET	5.0
1	1A	1058	G	5.0
47	1p	17	TYR	5.0
50	2s	35	SER	5.0
57	2y	40	C	5.0
38	1g	153	HIS	4.9
1	1A	2178	C	4.9
32	1a	1028	C	4.9
40	2i	72	GLY	4.9
23	21	2	SER	4.9
45	2n	6	LEU	4.9
44	2m	13	LYS	4.9
1	1A	2109	U	4.9
1	2A	2120	G	4.9
1	1A	1076	C	4.9
7	2H	51	ARG	4.9
57	1y	29	A	4.9
26	14	59	PHE	4.9
1	1A	2121	G	4.9
32	2a	1024	G	4.9
50	2s	13	ASP	4.9
21	2Z	153	SER	4.9
32	2a	1026	G	4.9
23	11	98	LEU	4.9
35	1d	167	GLY	4.9
54	1w	56	C	4.9
1	1A	1097	U	4.9
26	24	68	ARG	4.9
38	2g	79	ARG	4.9
41	1j	5	ARG	4.9
45	2n	31	ARG	4.9
57	1y	46	A	4.8
35	1d	168	ARG	4.8
6	2G	62	LEU	4.8
33	2b	118	LEU	4.8

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Mol	Chain	Res	Type	RSRZ
1	1A	1082	U	4.8
54	2w	45	U	4.8
34	2c	138	VAL	4.8
57	2y	13	C	4.8
7	2H	123	PHE	4.8
43	2l	64	TYR	4.8
32	1a	1040	U	4.8
41	2j	39	PRO	4.8
32	2a	1027	C	4.8
57	1y	61	C	4.8
38	2g	42	ILE	4.8
26	14	45	GLY	4.8
21	2Z	172	ALA	4.8
45	2n	10	ALA	4.8
44	2m	4	ILE	4.8
1	1A	2133	G	4.8
54	2w	28	G	4.8
57	2y	71	G	4.8
45	2n	29	ARG	4.8
52	2u	14	TRP	4.8
41	1j	40	LEU	4.8
54	1w	44	A	4.8
34	2c	198	VAL	4.8
41	1j	18	ALA	4.8
1	2A	2137	C	4.8
57	1y	28	G	4.7
35	2d	164	ALA	4.7
44	2m	42	ALA	4.7
21	2Z	5	LEU	4.7
49	2r	66	LEU	4.7
1	1A	2144	U	4.7
1	1A	1069	A	4.7
41	2j	13	HIS	4.7
40	2i	90	PRO	4.7
45	2n	15	LYS	4.7
36	2e	133	TYR	4.7
33	2b	48	MET	4.7
54	1w	66	C	4.7
57	1y	6	C	4.7
50	2s	69	HIS	4.7
32	2a	1030(D)	A	4.7
45	2n	53	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
1	1A	2166	G	4.7
1	1A	2128	C	4.7
1	2A	2136	C	4.7
43	2l	18	VAL	4.7
47	1p	48	TRP	4.7
26	14	54	GLY	4.7
1	1A	2135	A	4.7
1	2A	2170	A	4.7
12	2Q	104	PHE	4.7
33	2b	127	ILE	4.7
1	1A	2140	C	4.6
1	2A	888	C	4.6
32	1a	1030(A)	G	4.6
33	2b	101	MET	4.6
21	2Z	148	ASP	4.6
45	2n	57	ARG	4.6
1	2A	2156	G	4.6
1	2A	2181	G	4.6
32	1a	1023	G	4.6
33	2b	55	PHE	4.6
41	2j	88	LEU	4.6
1	2A	2144	U	4.6
1	1A	1100	C	4.6
1	1A	2143	C	4.6
1	2A	2178	C	4.6
40	2i	18	PHE	4.6
1	1A	1070	A	4.6
12	2Q	102	VAL	4.6
21	2Z	9	TYR	4.6
6	2G	60	LEU	4.6
14	2S	58	LEU	4.6
45	2n	44	LEU	4.6
1	1A	2108	C	4.6
50	2s	68	GLY	4.6
1	2A	2165	G	4.6
57	1y	7	G	4.6
29	27	46	VAL	4.6
1	1A	2158	A	4.6
54	2w	50	A	4.6
7	2H	128	PRO	4.6
57	1y	59	U	4.6
1	2A	2121	G	4.6

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Mol	Chain	Res	Type	RSRZ
34	2c	14	ILE	4.6
41	2j	38	ILE	4.6
1	2A	2177	C	4.5
38	1g	82	GLY	4.5
7	2H	159	GLU	4.5
34	1c	201	TYR	4.5
54	2w	67	G	4.5
33	2b	51	LEU	4.5
33	2b	70	PHE	4.5
33	2b	122	PHE	4.5
53	1v	24	A	4.5
34	1c	38	ARG	4.5
1	1A	2122	U	4.5
54	1w	13	C	4.5
57	1y	75	C	4.5
34	2c	60	ALA	4.5
32	2a	1032	G	4.5
21	2Z	1	MET	4.5
14	2S	37	ALA	4.5
1	2A	2125	G	4.5
7	2H	6	ARG	4.5
38	1g	154	TYR	4.5
44	2m	87	TYR	4.5
33	2b	201	ILE	4.5
41	2j	98	ILE	4.5
48	1q	36	ILE	4.5
45	2n	22	THR	4.5
1	1A	2167	U	4.5
57	1y	4	G	4.5
7	2H	103	LEU	4.5
11	2P	91	PHE	4.5
52	2u	11	GLY	4.5
5	2F	115	ALA	4.5
1	2A	2126	A	4.5
26	24	50	VAL	4.5
50	2s	16	LEU	4.5
32	1a	1037	C	4.5
40	2i	21	PRO	4.5
44	2m	57	ARG	4.5
35	1d	157	LEU	4.4
33	2b	105	PHE	4.4
40	2i	62	TYR	4.4

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Mol	Chain	Res	Type	RSRZ
1	1A	1066	U	4.4
40	2i	26	VAL	4.4
45	2n	50	LYS	4.4
57	2y	4	G	4.4
11	2P	140	ALA	4.4
41	1j	27	ALA	4.4
38	1g	78	ARG	4.4
34	2c	188	LEU	4.4
14	2S	29	PHE	4.4
1	2A	2166	G	4.4
54	1w	17	G	4.4
50	1s	51	VAL	4.4
34	2c	105	GLU	4.4
21	1Z	170	THR	4.4
42	2k	25	TYR	4.4
47	1p	41	PRO	4.4
36	2e	45	PHE	4.4
32	2a	1035	A	4.4
36	2e	8	GLU	4.4
57	1y	14	A	4.4
1	1A	2132	U	4.4
21	2Z	155	LEU	4.4
50	2s	30	LEU	4.4
45	2n	46	GLU	4.4
33	1b	123	ALA	4.3
34	2c	171	GLY	4.3
40	2i	43	ALA	4.3
6	2G	2	PRO	4.3
38	1g	85	TYR	4.3
57	1y	62	C	4.3
7	2H	115	VAL	4.3
21	2Z	128	VAL	4.3
40	2i	28	VAL	4.3
40	2i	109	VAL	4.3
1	2A	2148	G	4.3
32	2a	1030(C)	G	4.3
57	1y	19	U	4.3
7	2H	133	VAL	4.3
48	2q	23	VAL	4.3
50	2s	36	ARG	4.3
57	1y	18	G	4.3
40	1i	17	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
33	1b	211	ILE	4.3
7	2H	94	TYR	4.3
54	1w	30	G	4.3
34	2c	145	GLY	4.3
36	2e	115	VAL	4.3
32	2a	1030	C	4.3
34	2c	144	SER	4.3
11	2P	118	GLY	4.3
42	1k	25	TYR	4.3
1	2A	2153	G	4.3
1	1A	2137	C	4.3
40	2i	52	ALA	4.3
40	2i	106	ALA	4.3
40	2i	77	ILE	4.3
54	2w	56	C	4.3
57	1y	2	C	4.3
21	1Z	148	ASP	4.3
33	2b	164	VAL	4.3
50	2s	11	VAL	4.3
32	1a	1024	G	4.3
1	1A	2161	C	4.2
50	2s	63	THR	4.2
7	2H	145	ALA	4.2
41	2j	41	PRO	4.2
1	1A	2125	G	4.2
21	2Z	156	LYS	4.2
41	1j	23	ILE	4.2
26	14	55	ARG	4.2
34	2c	6	HIS	4.2
44	2m	53	VAL	4.2
40	2i	114	TYR	4.2
35	2d	2	GLY	4.2
57	1y	15	A	4.2
57	1y	58	A	4.2
44	2m	60	VAL	4.2
7	2H	102	ALA	4.2
26	24	59	PHE	4.2
34	2c	157	ILE	4.2
6	1G	139	LEU	4.2
54	1w	18	G	4.2
41	1j	10	GLY	4.2
1	2A	2169	A	4.2

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Mol	Chain	Res	Type	RSRZ
7	2H	43	VAL	4.2
33	1b	70	PHE	4.2
44	2m	84	ILE	4.2
50	2s	31	ILE	4.2
50	2s	39	THR	4.2
36	2e	131	ILE	4.1
21	2Z	91	LEU	4.1
34	1c	196	LEU	4.1
36	2e	114	GLY	4.1
54	1w	14	A	4.1
54	1w	31	C	4.1
50	2s	62	ILE	4.1
34	2c	57	ILE	4.1
32	1a	204	U	4.1
57	2y	45	U	4.1
41	2j	55	LYS	4.1
25	23	29	ARG	4.1
33	1b	188	ALA	4.1
50	1s	40	ILE	4.1
57	2y	27	A	4.1
41	2j	67	THR	4.1
1	1A	2151	G	4.1
11	2P	83	VAL	4.1
45	1n	25	VAL	4.1
45	2n	55	GLY	4.1
34	2c	124	ILE	4.1
6	2G	3	LEU	4.1
54	1w	23	A	4.1
57	2y	58	A	4.1
6	2G	29	TRP	4.1
50	2s	51	VAL	4.1
44	2m	68	GLY	4.1
32	1a	1034	G	4.1
33	2b	185	ILE	4.1
36	2e	76	ILE	4.1
1	2A	2161	C	4.1
54	1w	27	A	4.1
40	2i	65	VAL	4.1
52	2u	2	GLY	4.1
32	1a	1031	G	4.0
32	1a	1039	C	4.0
57	2y	63	C	4.0

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Mol	Chain	Res	Type	RSRZ
11	2P	79	ARG	4.0
38	2g	4	ARG	4.0
40	2i	86	VAL	4.0
1	2A	2109	U	4.0
1	1A	1093	G	4.0
32	2a	1021	G	4.0
40	2i	42	ARG	4.0
41	2j	34	VAL	4.0
57	2y	46	A	4.0
40	2i	105	ASP	4.0
41	1j	9	ARG	4.0
41	1j	35	SER	4.0
33	2b	203	GLY	4.0
35	1d	181	MET	4.0
1	1A	896	A	4.0
34	2c	5	ILE	4.0
40	2i	92	TYR	4.0
1	1A	2164	C	4.0
1	1A	2154	G	4.0
32	1a	1029	C	4.0
6	2G	137	GLU	4.0
1	2A	2157	G	4.0
20	2Y	90	LEU	4.0
32	2a	1001(A)	G	4.0
42	2k	49	GLY	4.0
29	17	47	ARG	4.0
21	2Z	50	GLN	4.0
21	2Z	8	TYR	4.0
1	2A	2175	C	3.9
33	2b	200	ILE	3.9
54	1w	7	G	3.9
54	1w	21	A	3.9
57	2y	5	G	3.9
34	1c	206	GLU	3.9
41	2j	64	GLU	3.9
41	2j	56	HIS	3.9
38	2g	84	ASN	3.9
6	2G	135	LEU	3.9
40	1i	47	LEU	3.9
43	2l	32	PHE	3.9
45	2n	12	ARG	3.9
1	2A	2164	C	3.9

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Mol	Chain	Res	Type	RSRZ
1	1A	1054	A	3.9
14	2S	33	LYS	3.9
31	29	16	VAL	3.9
44	2m	66	LEU	3.9
50	2s	49	ILE	3.9
34	2c	53	ALA	3.9
54	2w	73	U	3.9
26	24	29	PRO	3.9
7	2H	44	VAL	3.9
33	2b	216	SER	3.9
40	2i	79	LEU	3.9
50	2s	79	THR	3.9
32	2a	1020	U	3.9
1	1A	2138	C	3.9
34	2c	185	GLY	3.9
40	1i	80	GLY	3.9
43	2l	72	GLY	3.9
1	1A	1077	A	3.9
32	1a	1001	A	3.9
34	1c	70	VAL	3.9
38	2g	85	TYR	3.9
53	2v	13	A	3.9
31	29	13	LYS	3.9
34	2c	33	LEU	3.9
45	2n	51	GLY	3.9
20	2Y	75	ILE	3.9
38	1g	20	ASP	3.9
33	2b	232	PRO	3.9
1	1A	2136	C	3.9
54	2w	42	C	3.9
54	2w	69	C	3.9
7	2H	125	VAL	3.9
47	1p	39	TYR	3.9
50	2s	15	LEU	3.9
33	2b	163	PHE	3.8
40	2i	67	GLY	3.8
53	2v	23	A	3.8
45	2n	49	HIS	3.8
1	1A	1509	C	3.8
7	2H	144	VAL	3.8
12	2Q	32	TYR	3.8
26	24	42	PHE	3.8

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Mol	Chain	Res	Type	RSRZ
44	2m	12	ASN	3.8
51	1t	55	ILE	3.8
40	2i	45	ALA	3.8
21	2Z	76	LEU	3.8
41	2j	62	HIS	3.8
26	24	18	CYS	3.8
40	2i	93	ARG	3.8
51	2t	59	ALA	3.8
52	2u	13	ILE	3.8
50	2s	70	LYS	3.8
35	1d	180	GLY	3.8
21	2Z	59	LEU	3.8
45	2n	45	ARG	3.8
41	2j	48	THR	3.8
34	1c	189	ALA	3.8
36	2e	109	ILE	3.8
40	2i	110	GLU	3.8
50	1s	67	VAL	3.8
41	2j	87	THR	3.8
34	2c	109	PRO	3.8
39	2h	35	ILE	3.8
19	2X	92	LEU	3.8
36	2e	90	VAL	3.8
40	1i	65	VAL	3.8
41	1j	72	VAL	3.8
40	2i	49	PRO	3.8
47	1p	46	PRO	3.8
1	1A	2139	C	3.8
32	2a	1031	G	3.8
32	2a	1219	U	3.8
50	2s	29	ARG	3.8
57	2y	64	U	3.8
36	2e	12	LEU	3.8
38	2g	99	LEU	3.8
41	2j	44	VAL	3.8
41	2j	49	VAL	3.8
45	2n	13	THR	3.8
34	2c	71	ALA	3.7
40	2i	76	ALA	3.7
40	1i	8	GLY	3.7
32	2a	1018	C	3.7
33	2b	37	ASN	3.7

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Mol	Chain	Res	Type	RSRZ
34	2c	206	GLU	3.7
33	2b	81	VAL	3.7
34	2c	18	TRP	3.7
38	1g	26	PHE	3.7
34	1c	39	ILE	3.7
50	2s	53	ASN	3.7
57	2y	9	A	3.7
26	24	31	ILE	3.7
1	2A	2793	G	3.7
40	2i	13	ALA	3.7
45	1n	16	PHE	3.7
52	1u	13	ILE	3.7
1	2A	2132	U	3.7
50	2s	37	ARG	3.7
1	1A	2188	C	3.7
7	2H	2	SER	3.7
7	2H	7	LEU	3.7
39	2h	2	LEU	3.7
54	2w	61	C	3.7
57	2y	68	C	3.7
7	2H	13	LYS	3.7
34	2c	4	LYS	3.7
21	2Z	122	ARG	3.7
1	2A	652(U)	G	3.7
54	1w	67	G	3.7
40	2i	95	LYS	3.7
40	2i	6	GLY	3.7
32	2a	1039	C	3.7
57	2y	61	C	3.7
44	2m	3	ARG	3.7
57	1y	11	U	3.7
26	24	43	TYR	3.7
57	2y	67	G	3.7
26	24	39	CYS	3.7
26	24	66	SER	3.7
31	29	19	ARG	3.7
35	2d	156	GLU	3.7
38	2g	155	ARG	3.7
8	2I	107	VAL	3.7
21	1Z	139	VAL	3.7
57	1y	42	C	3.7
1	2A	2122	U	3.6

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Mol	Chain	Res	Type	RSRZ
50	2s	42	PRO	3.6
1	1A	2162	G	3.6
47	1p	6	LEU	3.6
21	2Z	152	ALA	3.6
33	1b	93	VAL	3.6
1	1A	1056	G	3.6
1	1A	2123	G	3.6
38	2g	78	ARG	3.6
54	1w	25	C	3.6
57	2y	12	U	3.6
33	2b	215	LEU	3.6
12	2Q	103	MET	3.6
35	2d	183	GLY	3.6
40	1i	18	PHE	3.6
1	1A	889	C	3.6
21	2Z	93	ASP	3.6
33	2b	183	PRO	3.6
50	1s	38	SER	3.6
21	2Z	140	ASP	3.6
33	2b	162	ILE	3.6
1	2A	652(T)	C	3.6
12	2Q	37	LEU	3.6
34	1c	113	ALA	3.6
34	1c	200	ALA	3.6
34	2c	200	ALA	3.6
50	1s	19	VAL	3.6
33	2b	39	ILE	3.6
31	29	20	HIS	3.6
40	2i	98	PRO	3.6
1	1A	888	C	3.6
33	2b	102	LEU	3.6
34	2c	52	LEU	3.6
20	2Y	55	TYR	3.6
34	2c	81	GLY	3.6
7	2H	141	VAL	3.6
33	2b	53	ARG	3.5
1	1A	278	A	3.5
25	23	60	GLU	3.5
50	2s	48	THR	3.5
57	1y	74	C	3.5
41	1j	7	LYS	3.5
44	2m	65	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
34	1c	193	TYR	3.5
51	1t	86	ARG	3.5
41	1j	96	ILE	3.5
41	1j	32	ALA	3.5
33	2b	31	TYR	3.5
1	1A	2165	G	3.5
1	1A	2168	G	3.5
26	24	69	LYS	3.5
51	2t	55	ILE	3.5
51	2t	63	ILE	3.5
57	1y	60	U	3.5
47	1p	42	ARG	3.5
21	1Z	141	VAL	3.5
33	2b	93	VAL	3.5
40	2i	53	VAL	3.5
43	1l	64	TYR	3.5
57	2y	6	C	3.5
34	1c	8	ILE	3.5
50	2s	10	PHE	3.5
40	2i	16	ARG	3.5
40	2i	39	GLY	3.5
44	2m	104	ARG	3.5
32	1a	79	G	3.5
36	1e	21	ALA	3.5
36	1e	95	ALA	3.5
34	1c	21	ARG	3.5
22	20	45	PHE	3.5
40	2i	81	ILE	3.5
11	2P	85	LEU	3.5
1	1A	2157	G	3.5
54	2w	7	G	3.5
57	2y	17	G	3.5
34	1c	179	ARG	3.5
1	2A	2108	C	3.5
34	1c	63	ASN	3.5
34	2c	159	GLY	3.5
36	2e	99	GLY	3.5
8	2I	75	LEU	3.5
14	2S	110	LEU	3.5
41	1j	21	GLN	3.5
32	2a	1202	G	3.5
33	1b	133	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
40	2i	4	TYR	3.4
43	2l	69	TYR	3.4
34	2c	202	ILE	3.4
41	1j	6	ILE	3.4
45	2n	16	PHE	3.4
54	1w	6	C	3.4
55	2x	47	U	3.4
19	2X	68	ARG	3.4
40	1i	46	ALA	3.4
33	1b	233	SER	3.4
27	15	60	VAL	3.4
41	1j	83	GLU	3.4
1	1A	1067	A	3.4
38	1g	4	ARG	3.4
40	1i	63	ILE	3.4
47	2p	19	ILE	3.4
51	2t	100	ILE	3.4
5	2F	32	LEU	3.4
41	2j	89	ASP	3.4
44	2m	70	LEU	3.4
34	2c	72	LYS	3.4
35	1d	23	GLY	3.4
35	2d	159	ARG	3.4
1	1A	1063	G	3.4
1	1A	2118	U	3.4
1	2A	2158	A	3.4
1	2A	2189	U	3.4
34	2c	101	LEU	3.4
44	2m	90	LEU	3.4
57	2y	60	U	3.4
32	1a	1030	C	3.4
40	1i	76	ALA	3.4
35	2d	198	VAL	3.4
34	2c	111	LEU	3.4
34	1c	146	ALA	3.4
3	2D	38	LYS	3.4
31	29	15	LYS	3.4
7	2H	82	GLY	3.4
8	2I	35	LEU	3.4
21	2Z	3	TYR	3.4
21	2Z	150	LEU	3.4
51	1t	84	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
40	2i	64	THR	3.4
38	2g	86	GLN	3.4
32	1a	1030(C)	G	3.4
32	2a	1149	C	3.4
57	1y	63	C	3.4
11	2P	125	VAL	3.4
33	2b	229	VAL	3.4
34	2c	77	ILE	3.4
7	2H	47	GLU	3.4
21	2Z	145	GLU	3.4
34	1c	68	VAL	3.4
40	2i	41	VAL	3.4
44	2m	92	HIS	3.4
52	2u	22	ARG	3.4
52	1u	2	GLY	3.3
6	2G	19	LEU	3.3
6	2G	90	LEU	3.3
7	2H	148	ILE	3.3
33	2b	222	ILE	3.3
33	2b	177	ALA	3.3
41	2j	68	HIS	3.3
52	2u	9	ARG	3.3
54	1w	15	A	3.3
1	2A	2107	C	3.3
50	1s	35	SER	3.3
54	2w	30	G	3.3
38	1g	27	ILE	3.3
12	2Q	5	ARG	3.3
38	2g	119	ARG	3.3
7	2H	45	VAL	3.3
35	2d	112	VAL	3.3
46	2o	60	VAL	3.3
32	1a	1007	C	3.3
57	1y	27	A	3.3
45	1n	17	LYS	3.3
14	2S	35	ILE	3.3
41	1j	45	ARG	3.3
41	2j	46	ARG	3.3
57	1y	26	G	3.3
26	14	57	GLU	3.3
21	2Z	4	ARG	3.3
40	1i	66	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
44	2m	80	ARG	3.3
51	1t	63	ILE	3.3
57	1y	40	C	3.3
52	2u	8	THR	3.3
7	2H	83	TYR	3.3
29	17	48	LYS	3.3
39	2h	65	TYR	3.3
50	2s	72	GLY	3.3
40	2i	107	ARG	3.3
41	1j	34	VAL	3.3
11	2P	88	LEU	3.3
38	1g	22	LEU	3.3
40	1i	79	LEU	3.3
21	1Z	146	ILE	3.3
1	2A	2105	C	3.3
21	2Z	51	ALA	3.3
39	2h	13	ILE	3.3
32	2a	1286	A	3.3
40	2i	61	ALA	3.3
22	10	3	HIS	3.3
20	1Y	1	MET	3.3
26	24	64	GLY	3.3
7	2H	95	ARG	3.3
11	2P	15	ARG	3.3
44	2m	64	TRP	3.3
44	1m	98	VAL	3.3
14	2S	84	GLN	3.3
23	11	82	LEU	3.3
45	2n	30	ALA	3.3
26	24	45	GLY	3.3
39	2h	130	GLY	3.3
29	27	47	ARG	3.3
42	2k	43	SER	3.3
1	2A	2833	G	3.2
37	1f	79	LEU	3.2
33	2b	227	GLY	3.2
1	2A	2140	C	3.2
33	2b	8	LYS	3.2
21	2Z	92	SER	3.2
26	24	25	TYR	3.2
50	2s	9	VAL	3.2
6	2G	136	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
21	2Z	69	THR	3.2
26	14	68	ARG	3.2
33	1b	61	LEU	3.2
40	1i	85	LEU	3.2
40	2i	20	ARG	3.2
41	2j	70	ARG	3.2
1	1A	2148	G	3.2
15	2T	52	ILE	3.2
21	2Z	133	ILE	3.2
31	29	12	ASP	3.2
9	2N	83	LYS	3.2
1	2A	2896	C	3.2
41	2j	59	SER	3.2
32	1a	1447	A	3.2
21	2Z	68	PRO	3.2
52	1u	21	TYR	3.2
14	2S	3	ARG	3.2
35	2d	168	ARG	3.2
12	2Q	22	LYS	3.2
34	1c	12	LEU	3.2
39	2h	112	LEU	3.2
41	1j	16	LEU	3.2
17	2V	92	THR	3.2
34	1c	57	ILE	3.2
20	2Y	5	MET	3.2
32	2a	1002	G	3.2
33	2b	90	MET	3.2
35	1d	179	GLU	3.2
54	1w	5	G	3.2
50	1s	4	SER	3.2
32	1a	1008	C	3.2
41	1j	41	PRO	3.2
1	1A	2119	A	3.2
1	2A	2173	A	3.2
18	1W	112	GLY	3.2
34	2c	180	ALA	3.2
45	1n	13	THR	3.2
1	2A	2180	U	3.2
7	2H	69	ARG	3.2
7	2H	97	ARG	3.2
40	1i	9	ARG	3.2
40	2i	128	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
57	1y	17	G	3.2
1	1A	1080	C	3.2
7	2H	26	VAL	3.2
32	2a	1001	A	3.2
34	2c	170	GLN	3.2
45	1n	8	GLU	3.2
40	1i	7	THR	3.2
1	2A	2102	U	3.2
14	2S	97	ARG	3.2
44	2m	88	ARG	3.2
1	2A	2805	G	3.2
7	2H	19	VAL	3.2
32	1a	1009	G	3.2
1	1A	2103	C	3.2
7	2H	171	LEU	3.2
33	2b	33	TYR	3.2
38	2g	22	LEU	3.2
40	1i	88	TYR	3.2
54	1w	1	G	3.2
38	2g	24	THR	3.2
41	1j	90	LEU	3.2
45	2n	4	LYS	3.2
47	1p	60	LEU	3.2
1	1A	2134	A	3.2
38	2g	26	PHE	3.2
1	1A	885	C	3.1
1	1A	1087	G	3.1
1	1A	1078	U	3.1
40	1i	37	PHE	3.1
34	1c	185	GLY	3.1
45	1n	15	LYS	3.1
21	2Z	173	ALA	3.1
44	2m	18	ALA	3.1
32	1a	1025	U	3.1
36	2e	89	ILE	3.1
32	2a	1017	G	3.1
57	2y	50	A	3.1
5	2F	114	VAL	3.1
17	2V	22	VAL	3.1
21	2Z	157	LEU	3.1
33	2b	132	LYS	3.1
48	1q	27	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	2A	2188	C	3.1
1	2A	1170	G	3.1
21	2Z	56	VAL	3.1
21	2Z	170	THR	3.1
27	25	58	LEU	3.1
34	1c	168	ALA	3.1
7	2H	142	GLY	3.1
38	1g	84	ASN	3.1
21	2Z	138	GLU	3.1
7	2H	92	ILE	3.1
35	2d	158	ILE	3.1
54	1w	42	C	3.1
54	1w	29	A	3.1
7	2H	53	GLU	3.1
11	2P	92	GLU	3.1
41	2j	92	THR	3.1
31	29	26	ILE	3.1
32	1a	1000	U	3.1
41	2j	91	PRO	3.1
4	1E	195	LEU	3.1
32	1a	1030(D)	A	3.1
32	1a	1286	A	3.1
7	2H	50	VAL	3.1
35	1d	133	VAL	3.1
40	1i	41	VAL	3.1
40	1i	109	VAL	3.1
40	2i	58	HIS	3.1
50	1s	14	HIS	3.1
21	1Z	104	PHE	3.1
32	2a	1040	U	3.1
47	1p	19	ILE	3.1
57	1y	45	U	3.1
41	2j	17	ASP	3.1
1	1A	2142	C	3.1
40	2i	40	LEU	3.1
7	2H	131	VAL	3.1
33	2b	113	HIS	3.1
45	2n	59	ALA	3.1
57	2y	44	A	3.0
1	1A	2106	G	3.0
36	2e	10	MET	3.0
19	1X	95	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
36	2e	138	ALA	3.0
40	2i	75	ASP	3.0
11	2P	78	PRO	3.0
45	2n	54	PRO	3.0
37	2f	92	LYS	3.0
41	2j	50	ILE	3.0
26	24	54	GLY	3.0
54	2w	18	G	3.0
6	2G	34	LEU	3.0
25	23	35	ARG	3.0
33	2b	88	ALA	3.0
34	2c	187	ALA	3.0
36	2e	94	ALA	3.0
26	14	69	LYS	3.0
34	2c	195	VAL	3.0
35	2d	166	LYS	3.0
52	2u	5	ASP	3.0
32	1a	344	A	3.0
33	1b	200	ILE	3.0
40	2i	74	ILE	3.0
5	2F	7	TYR	3.0
6	2G	115	ARG	3.0
40	2i	78	LYS	3.0
12	2Q	129	THR	3.0
40	2i	47	LEU	3.0
40	2i	85	LEU	3.0
54	2w	39	G	3.0
11	2P	101	VAL	3.0
20	2Y	45	VAL	3.0
34	1c	138	VAL	3.0
36	2e	82	VAL	3.0
39	2h	93	VAL	3.0
32	1a	999	C	3.0
1	1A	271(K)	U	3.0
54	1w	45	U	3.0
40	2i	88	TYR	3.0
12	2Q	117	ALA	3.0
17	2V	94	LEU	3.0
41	1j	64	GLU	3.0
1	1A	2104	G	3.0
1	1A	2127	G	3.0
57	2y	10	G	3.0

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Mol	Chain	Res	Type	RSRZ
21	2Z	143	GLY	3.0
31	29	33	LYS	3.0
40	2i	22	GLY	3.0
41	2j	52	GLY	3.0
33	2b	152	PHE	3.0
35	2d	5	ILE	3.0
54	2w	11	U	3.0
33	2b	148	TYR	3.0
11	2P	115	LEU	3.0
35	1d	21	LEU	3.0
43	2l	68	ALA	3.0
37	1f	9	VAL	3.0
38	2g	13	GLN	3.0
39	1h	93	VAL	3.0
40	2i	115	GLY	3.0
32	2a	1023	G	3.0
41	2j	86	MET	3.0
1	1A	886	C	3.0
1	1A	1083	U	3.0
6	2G	39	ILE	3.0
12	2Q	65	PHE	3.0
34	1c	14	ILE	3.0
17	2V	93	GLU	3.0
44	1m	27	LYS	3.0
38	1g	16	LEU	3.0
33	2b	97	TRP	3.0
41	1j	70	ARG	3.0
44	2m	6	GLY	3.0
33	2b	184	VAL	2.9
41	2j	23	ILE	2.9
32	2a	1003	G	2.9
54	1w	26	G	2.9
35	1d	147	ALA	2.9
7	1H	174	GLY	2.9
50	2s	65	ASN	2.9
7	2H	107	VAL	2.9
38	1g	17	VAL	2.9
14	2S	34	HIS	2.9
4	2E	51	PHE	2.9
21	2Z	44	PHE	2.9
36	2e	84	PHE	2.9
7	2H	132	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
32	1a	1006	C	2.9
33	2b	77	ALA	2.9
33	2b	92	TYR	2.9
47	1p	38	TYR	2.9
34	2c	183	ASP	2.9
38	2g	105	VAL	2.9
54	1w	9	A	2.9
54	2w	27	A	2.9
6	2G	86	MET	2.9
12	2Q	19	GLY	2.9
1	2A	2142	C	2.9
7	2H	67	LEU	2.9
7	2H	106	THR	2.9
17	2V	35	LEU	2.9
41	1j	85	LEU	2.9
45	1n	14	PRO	2.9
51	1t	62	LEU	2.9
31	29	24	TYR	2.9
6	1G	136	ARG	2.9
38	2g	41	ARG	2.9
44	2m	17	VAL	2.9
40	1i	81	ILE	2.9
7	2H	172	LYS	2.9
7	2H	20	ALA	2.9
14	2S	32	LEU	2.9
26	24	27	THR	2.9
35	2d	176	LEU	2.9
41	2j	26	ALA	2.9
47	1p	22	THR	2.9
40	1i	110	GLU	2.9
48	2q	19	VAL	2.9
50	1s	58	VAL	2.9
1	2A	2792	G	2.9
32	1a	78	G	2.9
54	1w	39	G	2.9
57	2y	49	G	2.9
35	2d	146	ILE	2.9
9	2N	116	LEU	2.9
12	2Q	121	ALA	2.9
34	1c	32	LEU	2.9
34	2c	50	ALA	2.9
34	2c	87	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
40	2i	55	ALA	2.9
21	2Z	46	LYS	2.9
32	2a	1019	C	2.9
50	1s	52	TYR	2.9
36	2e	105	VAL	2.9
50	1s	41	VAL	2.9
1	2A	2162	G	2.9
54	1w	32	U	2.9
57	1y	10	G	2.9
57	2y	7	G	2.9
32	2a	1250	A	2.9
51	1t	80	ARG	2.9
53	1v	14	A	2.9
54	2w	44	A	2.9
6	2G	133	LEU	2.9
23	11	97	LEU	2.9
33	2b	135	GLN	2.9
34	2c	47	LEU	2.9
35	1d	120	LEU	2.9
41	2j	21	GLN	2.9
36	2e	100	VAL	2.8
44	2m	61	GLU	2.8
34	2c	190	ARG	2.8
6	2G	103	LEU	2.8
33	1b	19	HIS	2.8
36	2e	21	ALA	2.8
38	2g	117	ALA	2.8
41	1j	20	ALA	2.8
34	2c	115	LEU	2.8
18	2W	112	GLY	2.8
21	2Z	147	GLY	2.8
26	14	32	TYR	2.8
34	1c	48	TYR	2.8
34	2c	51	GLY	2.8
38	2g	115	ARG	2.8
40	1i	28	VAL	2.8
40	1i	108	VAL	2.8
1	1A	2105	C	2.8
26	24	7	PRO	2.8
32	2a	1150	U	2.8
34	1c	186	PHE	2.8
26	14	18	CYS	2.8

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Mol	Chain	Res	Type	RSRZ
34	2c	149	ALA	2.8
34	2c	189	ALA	2.8
33	2b	69	LEU	2.8
42	2k	31	THR	2.8
38	1g	81	GLY	2.8
40	1i	20	ARG	2.8
52	1u	9	ARG	2.8
33	2b	230	VAL	2.8
1	1A	2163	C	2.8
1	2A	2143	C	2.8
32	1a	841	U	2.8
32	2a	202	U	2.8
33	2b	68	ILE	2.8
39	2h	111	ILE	2.8
40	2i	59	PHE	2.8
33	2b	75	LYS	2.8
40	2i	50	LEU	2.8
54	2w	14	A	2.8
1	2A	2141	G	2.8
34	2c	201	TYR	2.8
41	1j	97	GLU	2.8
7	2H	10	PRO	2.8
7	2H	12	PRO	2.8
22	20	5	LYS	2.8
40	1i	59	PHE	2.8
1	1A	1092	C	2.8
35	2d	82	ALA	2.8
41	1j	26	ALA	2.8
31	29	22	ARG	2.8
34	2c	11	ARG	2.8
47	1p	13	HIS	2.8
21	1Z	133	ILE	2.8
26	24	44	THR	2.8
35	2d	160	GLN	2.8
44	1m	24	GLY	2.8
50	1s	39	THR	2.8
35	1d	163	GLU	2.8
41	2j	19	SER	2.8
8	2I	82	ARG	2.8
12	2Q	109	VAL	2.8
39	2h	61	VAL	2.8
54	2w	23	A	2.8

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Mol	Chain	Res	Type	RSRZ
9	2N	10	GLU	2.8
34	1c	65	ALA	2.8
43	2l	56	ALA	2.8
32	1a	1033	G	2.8
54	1w	28	G	2.8
41	1j	17	ASP	2.8
26	24	10	VAL	2.7
40	2i	31	GLN	2.7
43	2l	55	VAL	2.7
44	2m	67	GLU	2.7
44	2m	101	GLN	2.7
48	2q	9	VAL	2.7
50	2s	41	VAL	2.7
1	2A	272(A)	U	2.7
14	2S	36	TYR	2.7
34	2c	13	GLY	2.7
34	2c	23	TYR	2.7
35	1d	138	TYR	2.7
7	2H	89	ILE	2.7
51	1t	68	LYS	2.7
7	2H	88	LEU	2.7
33	1b	187	LEU	2.7
33	1b	215	LEU	2.7
40	2i	99	LEU	2.7
1	2A	2100	G	2.7
1	2A	2106	G	2.7
32	2a	1061	G	2.7
1	2A	652(V)	C	2.7
38	1g	34	GLY	2.7
50	1s	72	GLY	2.7
8	1I	26	ALA	2.7
29	17	45	ALA	2.7
33	2b	34	ALA	2.7
33	2b	58	ILE	2.7
34	2c	15	THR	2.7
40	1i	10	ARG	2.7
40	1i	64	THR	2.7
41	2j	51	ARG	2.7
50	1s	75	ALA	2.7
11	1P	105	LEU	2.7
12	2Q	34	LEU	2.7
50	2s	22	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
51	1t	89	ARG	2.7
52	2u	15	ARG	2.7
53	2v	14	A	2.7
50	1s	13	ASP	2.7
22	20	3	HIS	2.7
33	2b	76	GLN	2.7
14	2S	57	LYS	2.7
45	2n	14	PRO	2.7
40	2i	104	ARG	2.7
14	2S	82	ILE	2.7
36	1e	109	ILE	2.7
40	2i	94	ALA	2.7
42	2k	57	THR	2.7
50	1s	16	LEU	2.7
38	2g	33	ASP	2.7
41	2j	7	LYS	2.7
47	1p	59	TRP	2.7
32	2a	1028	C	2.7
7	2H	49	VAL	2.7
34	1c	198	VAL	2.7
34	1c	207	VAL	2.7
32	2a	1022	G	2.7
54	2w	22	G	2.7
1	1A	2102	U	2.7
38	2g	36	LYS	2.7
34	1c	33	LEU	2.7
34	2c	39	ILE	2.7
41	1j	100	THR	2.7
1	1A	2173	A	2.7
11	2P	93	GLY	2.7
50	2s	66	MET	2.7
52	1u	11	GLY	2.7
33	2b	220	ASP	2.7
54	1w	41	U	2.7
57	2y	11	U	2.7
16	2U	88	ILE	2.7
33	1b	214	ILE	2.7
33	2b	223	ILE	2.7
35	2d	186	LEU	2.7
41	1j	11	PHE	2.7
41	1j	65	LEU	2.7
44	2m	9	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
47	1p	73	LEU	2.7
51	1t	53	LEU	2.7
54	1w	22	G	2.7
33	2b	9	GLU	2.7
44	2m	21	TYR	2.7
48	2q	42	TYR	2.7
34	2c	16	ARG	2.7
6	2G	27	ASN	2.7
41	1j	99	LYS	2.7
1	2A	2172	U	2.7
7	2H	32	GLU	2.7
41	2j	81	THR	2.7
36	2e	119	LEU	2.7
57	1y	73	U	2.7
21	2Z	171	ILE	2.7
6	2G	12	TYR	2.7
34	2c	3	ASN	2.7
34	2c	78	GLY	2.7
32	2a	1014	A	2.6
7	2H	17	VAL	2.6
33	1b	136	VAL	2.6
21	1Z	150	LEU	2.6
32	1a	202	U	2.6
44	1m	122	LYS	2.6
35	2d	162	LEU	2.6
38	2g	12	LEU	2.6
54	1w	62	C	2.6
55	2x	1	C	2.6
57	2y	70	C	2.6
7	2H	174	GLY	2.6
7	2H	8	PRO	2.6
14	2S	92	TYR	2.6
47	2p	41	PRO	2.6
40	2i	3	GLN	2.6
21	2Z	28	MET	2.6
32	2a	485	G	2.6
35	2d	139	ARG	2.6
51	1t	14	LYS	2.6
52	2u	6	ARG	2.6
35	1d	104	VAL	2.6
1	1A	229	A	2.6
7	2H	165	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
34	2c	24	ALA	2.6
40	2i	46	ALA	2.6
54	2w	38	A	2.6
57	1y	9	A	2.6
38	1g	124	LEU	2.6
39	1h	2	LEU	2.6
41	2j	31	GLY	2.6
41	1j	95	GLU	2.6
54	1w	2	C	2.6
40	1i	36	TYR	2.6
40	2i	125	TYR	2.6
34	2c	142	MET	2.6
1	1A	1062	G	2.6
32	2a	1177	G	2.6
11	2P	141	ALA	2.6
33	2b	186	ALA	2.6
43	2l	43	VAL	2.6
45	2n	48	ALA	2.6
47	1p	7	ALA	2.6
50	1s	68	GLY	2.6
1	1A	2172	U	2.6
9	2N	112	LEU	2.6
23	1l	94	LEU	2.6
25	23	28	LEU	2.6
32	2a	1005	A	2.6
32	2a	1016	A	2.6
35	1d	11	LEU	2.6
15	2T	22	PHE	2.6
38	2g	43	PHE	2.6
40	1i	33	PHE	2.6
34	2c	199	LYS	2.6
44	2m	27	LYS	2.6
26	14	43	TYR	2.6
12	2Q	97	VAL	2.6
33	1b	15	VAL	2.6
42	2k	86	GLY	2.6
34	2c	17	ASP	2.6
38	1g	59	LEU	2.6
43	2l	93	LEU	2.6
44	2m	16	ASP	2.6
51	2t	72	LEU	2.6
52	1u	14	TRP	2.6

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Mol	Chain	Res	Type	RSRZ
7	2H	29	PRO	2.6
33	2b	64	ARG	2.6
35	2d	110	PHE	2.6
41	2j	37	PRO	2.6
19	2X	69	TYR	2.6
33	2b	95	GLN	2.6
6	2G	50	ALA	2.6
6	2G	70	VAL	2.6
37	2f	6	VAL	2.6
38	2g	152	ALA	2.6
40	1i	122	ALA	2.6
40	2i	83	ARG	2.6
44	2m	43	THR	2.6
21	2Z	95	PRO	2.6
32	2a	204	U	2.6
40	1i	90	PRO	2.6
6	2G	114	ILE	2.6
32	2a	1220	G	2.6
32	2a	1180	A	2.6
1	2A	2804	C	2.6
40	1i	57	GLY	2.6
41	2j	93	GLY	2.6
45	1n	41	ARG	2.6
52	2u	10	ARG	2.6
42	1k	15	ALA	2.6
21	1Z	100	VAL	2.6
26	24	56	VAL	2.6
33	1b	71	VAL	2.6
35	2d	157	LEU	2.6
39	2h	101	PRO	2.6
44	1m	90	LEU	2.6
57	1y	65	U	2.6
21	2Z	137	ILE	2.6
35	2d	206	PHE	2.6
39	1h	35	ILE	2.6
41	2j	96	ILE	2.6
11	2P	76	LYS	2.6
1	1A	2156	G	2.6
41	2j	9	ARG	2.6
1	1A	2185	C	2.6
1	2A	885	C	2.6
8	1I	41	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
26	24	57	GLU	2.6
32	2a	1116	C	2.6
33	2b	62	ALA	2.5
35	2d	163	GLU	2.6
47	1p	69	THR	2.5
51	1t	59	ALA	2.5
51	1t	67	ALA	2.5
33	1b	229	VAL	2.5
38	2g	21	VAL	2.5
35	1d	135	LEU	2.5
41	1j	37	PRO	2.5
41	2j	24	VAL	2.5
12	2Q	63	LYS	2.5
32	2a	1532	U	2.5
21	1Z	120	ILE	2.5
40	2i	124	GLN	2.5
34	2c	205	GLY	2.5
21	2Z	94	GLU	2.5
38	2g	123	GLU	2.5
50	1s	27	GLU	2.5
32	1a	1004	A	2.5
40	1i	62	TYR	2.5
44	1m	87	TYR	2.5
7	2H	33	LEU	2.5
26	24	9	LEU	2.5
34	2c	12	LEU	2.5
46	1o	57	LEU	2.5
1	2A	2118	U	2.5
21	2Z	48	PHE	2.5
35	2d	70	ILE	2.5
34	1c	98	ASN	2.5
47	1p	80	PHE	2.5
47	2p	9	PHE	2.5
7	2H	77	LYS	2.5
34	2c	22	TRP	2.5
11	2P	110	TYR	2.5
32	2a	1130	A	2.5
38	2g	44	TYR	2.5
42	1k	89	ALA	2.5
7	2H	169	VAL	2.5
33	2b	197	VAL	2.5
35	1d	112	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
50	2s	81	ARG	2.5
1	2A	2803	C	2.5
57	2y	48	C	2.5
26	24	65	ASP	2.5
40	2i	54	ASP	2.5
41	2j	36	GLY	2.5
44	2m	100	GLY	2.5
24	22	8	LYS	2.5
36	2e	9	LYS	2.5
7	2H	41	MET	2.5
5	1F	17	ARG	2.5
33	2b	131	PRO	2.5
34	2c	65	ALA	2.5
6	2G	149	VAL	2.5
21	1Z	154	ASP	2.5
21	2Z	70	LEU	2.5
20	2Y	22	GLY	2.5
38	2g	153	HIS	2.5
1	1A	2101	G	2.5
1	1A	2149	G	2.5
20	2Y	60	PHE	2.5
38	1g	47	CYS	2.5
40	1i	3	GLN	2.5
21	2Z	60	GLU	2.5
41	1j	60	ARG	2.5
12	2Q	114	ALA	2.5
50	2s	32	LYS	2.5
6	1G	152	LEU	2.5
7	2H	78	GLY	2.5
21	1Z	99	TYR	2.5
34	2c	64	VAL	2.5
39	2h	119	LEU	2.5
41	2j	69	ASN	2.5
46	2o	69	TYR	2.5
51	2t	101	GLY	2.5
51	2t	73	HIS	2.5
32	1a	1020	U	2.5
1	1A	1053	C	2.5
34	2c	143	GLU	2.5
36	1e	6	PHE	2.5
35	1d	33	MET	2.5
35	1d	159	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
43	2l	65	GLU	2.5
1	2A	2152	G	2.5
50	1s	53	ASN	2.5
6	2G	28	VAL	2.5
11	2P	105	LEU	2.5
21	2Z	47	VAL	2.5
40	1i	117	HIS	2.5
45	2n	8	GLU	2.5
6	2G	153	ARG	2.5
34	2c	85	ARG	2.5
45	2n	26	ARG	2.5
1	1A	2790	A	2.5
1	2A	2176	A	2.5
36	2e	11	ILE	2.5
1	2A	2183	C	2.5
32	2a	1114	C	2.5
54	1w	68	C	2.5
54	2w	66	C	2.5
41	1j	73	ASP	2.5
1	1A	2100	G	2.5
1	2A	2149	G	2.5
12	2Q	44	ALA	2.5
32	1a	1032	G	2.5
32	2a	1224	G	2.5
33	2b	85	ALA	2.5
51	1t	66	ALA	2.5
7	2H	158	HIS	2.4
5	2F	33	LEU	2.4
7	1H	7	LEU	2.4
37	1f	61	LEU	2.4
40	2i	96	LEU	2.4
41	2j	29	ARG	2.4
42	1k	84	VAL	2.4
42	2k	14	VAL	2.4
51	1t	58	LYS	2.4
21	2Z	66	SER	2.4
33	2b	17	PHE	2.4
34	1c	203	PHE	2.4
44	2m	78	ILE	2.4
51	2t	41	ILE	2.4
21	2Z	87	ASP	2.4
50	1s	66	MET	2.4

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Mol	Chain	Res	Type	RSRZ
11	2P	84	ASN	2.4
15	2T	55	ASN	2.4
38	2g	88	PRO	2.4
34	2c	21	ARG	2.4
40	1i	45	ALA	2.4
51	1t	79	ARG	2.4
11	2P	99	LEU	2.4
39	1h	133	LEU	2.4
26	24	33	VAL	2.4
6	2G	49	ASP	2.4
48	2q	36	ILE	2.4
6	2G	155	MET	2.4
21	2Z	98	MET	2.4
6	2G	132	ASN	2.4
46	1o	89	GLY	2.4
50	1s	18	LYS	2.4
32	1a	1531	A	2.4
7	2H	150	ALA	2.4
11	2P	127	ALA	2.4
14	2S	55	ALA	2.4
45	1n	59	ALA	2.4
54	1w	40	C	2.4
54	1w	48	C	2.4
14	2S	48	LEU	2.4
4	2E	87	GLU	2.4
5	2F	36	VAL	2.4
6	2G	92	VAL	2.4
8	1I	136	VAL	2.4
1	1A	1963	U	2.4
38	2g	30	ILE	2.4
40	1i	116	LYS	2.4
50	1s	31	ILE	2.4
50	2s	28	LYS	2.4
5	2F	172	TRP	2.4
6	2G	100	TRP	2.4
40	1i	42	ARG	2.4
51	2t	83	ARG	2.4
52	1u	15	ARG	2.4
52	1u	22	ARG	2.4
33	2b	38	GLY	2.4
34	2c	197	GLY	2.4
40	2i	123	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
34	1c	60	ALA	2.4
1	2A	2103	C	2.4
19	2X	95	LEU	2.4
21	2Z	142	SER	2.4
34	1c	204	LEU	2.4
37	1f	83	ASP	2.4
41	2j	35	SER	2.4
5	2F	105	VAL	2.4
12	2Q	106	VAL	2.4
33	2b	71	VAL	2.4
33	2b	112	VAL	2.4
34	2c	106	VAL	2.4
35	1d	170	VAL	2.4
11	2P	65	ARG	2.4
36	2e	60	TYR	2.4
11	2P	1	MET	2.4
20	2Y	89	PHE	2.4
33	1b	101	MET	2.4
41	1j	39	PRO	2.4
11	2P	94	GLU	2.4
47	1p	16	HIS	2.4
45	1n	10	ALA	2.4
7	1H	2	SER	2.4
35	1d	152	SER	2.4
51	2t	99	LEU	2.4
36	2e	107	ARG	2.4
48	2q	92	ARG	2.4
51	1t	22	ARG	2.4
54	1w	58	A	2.4
26	14	56	VAL	2.4
34	1c	64	VAL	2.4
43	2l	90	VAL	2.4
25	23	27	GLY	2.4
34	2c	63	ASN	2.4
6	2G	11	TYR	2.4
48	2q	95	TYR	2.4
50	1s	64	GLU	2.4
40	1i	21	PRO	2.4
50	2s	44	MET	2.4
35	2d	195	ALA	2.4
21	2Z	79	ARG	2.4
34	2c	172	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
35	2d	49	ARG	2.4
33	2b	98	LEU	2.4
8	1I	142	VAL	2.4
21	1Z	105	VAL	2.4
35	1d	198	VAL	2.4
57	1y	44	A	2.4
4	2E	1	MET	2.4
7	2H	4	ILE	2.4
28	26	54	ILE	2.4
41	1j	50	ILE	2.4
35	1d	110	PHE	2.4
41	1j	62	HIS	2.4
39	2h	104	ARG	2.4
47	1p	68	ASP	2.4
50	2s	24	ALA	2.4
38	1g	56	GLN	2.4
40	1i	31	GLN	2.4
21	2Z	125	LEU	2.4
32	2a	1011	G	2.3
34	1c	78	GLY	2.3
34	2c	155	GLY	2.3
40	2i	100	GLY	2.3
23	1I	49	VAL	2.3
33	2b	136	VAL	2.3
38	2g	135	VAL	2.3
1	1A	1088	A	2.3
32	1a	1137	C	2.3
54	2w	29	A	2.3
11	2P	90	ARG	2.3
33	2b	130	ARG	2.3
34	2c	59	ARG	2.3
38	1g	42	ILE	2.3
38	2g	120	ILE	2.3
35	1d	38	TYR	2.3
45	2n	52	GLN	2.3
21	1Z	169	GLU	2.3
34	1c	35	GLU	2.3
50	2s	64	GLU	2.3
4	2E	181	LEU	2.3
9	1N	138	LEU	2.3
20	1Y	14	LEU	2.3
21	2Z	64	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
33	2b	196	LEU	2.3
44	2m	56	LEU	2.3
45	2n	47	LEU	2.3
27	25	60	VAL	2.3
32	2a	1009	G	2.3
43	2l	39	VAL	2.3
31	29	30	PRO	2.3
33	2b	60	ASP	2.3
42	1k	96	ARG	2.3
1	1A	1075	C	2.3
1	1A	1086	A	2.3
4	2E	176	ILE	2.3
40	1i	113	LYS	2.3
41	2j	18	ALA	2.3
34	1c	41	GLY	2.3
34	2c	178	LEU	2.3
24	22	7	ARG	2.3
6	2G	35	GLU	2.3
21	2Z	2	GLU	2.3
26	24	53	GLU	2.3
39	2h	81	HIS	2.3
45	1n	49	HIS	2.3
50	2s	43	GLU	2.3
8	2I	142	VAL	2.3
21	2Z	65	GLN	2.3
24	22	63	VAL	2.3
36	2e	20	GLN	2.3
21	2Z	23	LYS	2.3
42	1k	83	ILE	2.3
6	2G	102	PHE	2.3
32	1a	1149	C	2.3
1	2A	2801(A)	A	2.3
6	2G	61	ALA	2.3
21	1Z	152	ALA	2.3
33	2b	94	ASN	2.3
34	1c	15	THR	2.3
34	1c	145	GLY	2.3
36	2e	16	THR	2.3
6	1G	135	LEU	2.3
12	2Q	6	ARG	2.3
25	23	30	ARG	2.3
33	2b	96	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
34	1c	52	LEU	2.3
34	2c	204	LEU	2.3
35	2d	73	ARG	2.3
36	2e	14	ARG	2.3
13	2R	69	ASP	2.3
26	14	46	GLN	2.3
50	1s	12	ASP	2.3
43	2l	54	LYS	2.3
21	2Z	71	VAL	2.3
21	2Z	146	ILE	2.3
35	2d	185	PHE	2.3
8	2I	59	ALA	2.3
1	2A	883	G	2.3
26	24	58	ARG	2.3
35	2d	147	ALA	2.3
33	1b	148	TYR	2.3
33	2b	190	THR	2.3
45	1n	34	TYR	2.3
52	1u	17	THR	2.3
57	1y	70	C	2.3
54	2w	21	A	2.3
38	2g	136	LYS	2.3
49	1r	31	LEU	2.3
6	2G	159	VAL	2.3
32	2a	1148	U	2.3
11	2P	109	GLY	2.3
38	2g	34	GLY	2.3
39	2h	122	ARG	2.3
5	2F	21	ALA	2.3
33	1b	152	PHE	2.3
34	2c	48	TYR	2.3
38	1g	44	TYR	2.3
24	22	60	LEU	2.3
33	2b	121	LEU	2.3
34	2c	69	HIS	2.3
36	2e	43	LEU	2.3
38	2g	38	LEU	2.3
11	2P	145	PRO	2.3
33	1b	30	ARG	2.3
35	1d	122	ARG	2.3
35	2d	140	VAL	2.3
35	2d	148	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
7	2H	25	LYS	2.3
29	27	1	MET	2.3
14	2S	109	GLY	2.3
17	1V	101	GLY	2.3
6	2G	138	GLN	2.3
42	2k	21	ILE	2.3
33	1b	55	PHE	2.3
42	2k	89	ALA	2.3
42	2k	125	PHE	2.3
26	24	40	HIS	2.3
21	2Z	29	TYR	2.3
37	2f	4	TYR	2.3
44	1m	21	TYR	2.3
54	2w	6	C	2.3
7	2H	175	LYS	2.2
33	1b	75	LYS	2.2
35	1d	166	LYS	2.2
36	2e	25	ARG	2.2
37	1f	46	ARG	2.2
51	1t	83	ARG	2.2
51	1t	98	PRO	2.2
32	1a	1021	G	2.2
32	1a	1138	G	2.2
32	2a	1156	G	2.2
6	2G	26	GLN	2.2
8	2I	104	GLN	2.2
34	1c	170	GLN	2.2
41	1j	19	SER	2.2
45	2n	32	SER	2.2
9	2N	85	ILE	2.2
37	1f	8	ILE	2.2
6	1G	80	PHE	2.2
21	2Z	88	PHE	2.2
50	1s	50	ALA	2.2
7	2H	124	GLU	2.2
33	1b	97	TRP	2.2
33	1b	126	GLU	2.2
36	2e	81	GLU	2.2
36	2e	111	GLU	2.2
44	2m	69	GLU	2.2
7	2H	101	ARG	2.2
12	2Q	130	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
15	2T	129	ARG	2.2
34	2c	54	ARG	2.2
35	2d	21	LEU	2.2
45	1n	6	LEU	2.2
45	1n	11	LYS	2.2
45	2n	19	ARG	2.2
8	1I	137	PRO	2.2
32	2a	1179	A	2.2
34	2c	80	GLY	2.2
34	2c	158	GLY	2.2
17	2V	72	VAL	2.2
21	2Z	58	VAL	2.2
33	2b	7	VAL	2.2
40	1i	86	VAL	2.2
42	1k	14	VAL	2.2
15	2T	67	SER	2.2
1	1A	1176	G	2.2
1	2A	892	G	2.2
41	1j	25	GLU	2.2
54	2w	26	G	2.2
7	2H	9	ILE	2.2
33	1b	163	PHE	2.2
40	1i	82	ALA	2.2
41	2j	54	PHE	2.2
35	2d	132	ARG	2.2
6	1G	7	LEU	2.2
35	2d	96	LEU	2.2
37	2f	59	TYR	2.2
42	2k	50	TYR	2.2
14	1S	60	GLY	2.2
44	1m	26	GLY	2.2
1	2A	645	C	2.2
1	2A	1041	C	2.2
20	2Y	91	GLU	2.2
21	2Z	162	GLU	2.2
32	2a	999	C	2.2
57	2y	69	C	2.2
3	2D	113	VAL	2.2
54	1w	24	A	2.2
12	2Q	66	ILE	2.2
30	28	16	ILE	2.2
34	2c	134	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
38	2g	76	ARG	2.2
50	1s	69	HIS	2.2
51	1t	76	ALA	2.2
52	1u	6	ARG	2.2
10	2O	14	THR	2.2
57	1y	67	G	2.2
6	2G	43	LEU	2.2
10	2O	101	PRO	2.2
19	1X	13	LEU	2.2
49	2r	85	LEU	2.2
34	2c	167	TRP	2.2
38	2g	28	ASN	2.2
44	2m	8	GLU	2.2
30	28	15	LYS	2.2
35	2d	20	TYR	2.2
1	2A	2794	C	2.2
16	2U	8	VAL	2.2
22	20	66	VAL	2.2
25	23	47	VAL	2.2
25	23	59	VAL	2.2
26	14	50	VAL	2.2
32	2a	1038	C	2.2
38	2g	3	ARG	2.2
39	2h	26	VAL	2.2
50	2s	60	VAL	2.2
39	2h	80	ILE	2.2
50	1s	10	PHE	2.2
52	1u	8	THR	2.2
40	2i	87	GLN	2.2
14	2S	59	LYS	2.2
21	2Z	130	PRO	2.2
33	1b	196	LEU	2.2
34	1c	43	LEU	2.2
41	1j	22	LYS	2.2
45	1n	39	LEU	2.2
48	2q	22	LEU	2.2
49	1r	78	LEU	2.2
52	1u	23	PRO	2.2
14	2S	67	ARG	2.2
41	2j	5	ARG	2.2
41	2j	45	ARG	2.2
45	2n	41	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
46	1o	88	ARG	2.2
14	2S	46	VAL	2.2
38	2g	31	MET	2.2
38	2g	118	VAL	2.2
41	1j	68	HIS	2.2
49	1r	39	VAL	2.2
51	1t	85	MET	2.2
1	2A	1043	C	2.2
25	23	25	ALA	2.2
34	1c	105	GLU	2.2
38	1g	39	ALA	2.2
50	2s	27	GLU	2.2
5	2F	82	ILE	2.2
8	1I	79	ILE	2.2
8	2I	88	ILE	2.2
36	2e	118	ILE	2.2
37	1f	52	ILE	2.2
40	2i	127	LYS	2.2
46	1o	36	ILE	2.2
1	1A	1084	A	2.2
3	2D	177	LEU	2.2
11	2P	106	LEU	2.2
12	2Q	2	LEU	2.2
24	22	61	LEU	2.2
33	2b	149	LEU	2.2
35	2d	194	LEU	2.2
38	1g	99	LEU	2.2
50	1s	30	LEU	2.2
50	2s	82	GLY	2.2
32	2a	1178	G	2.2
52	2u	18	TYR	2.2
7	2H	30	LYS	2.2
10	2O	102	VAL	2.2
31	29	25	VAL	2.2
33	1b	230	VAL	2.2
34	1c	120	VAL	2.2
34	2c	153	VAL	2.2
44	2m	82	MET	2.2
15	2T	48	ILE	2.2
32	2a	1037	C	2.2
36	1e	118	ILE	2.2
41	2j	100	THR	2.2

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Mol	Chain	Res	Type	RSRZ
21	2Z	82	ARG	2.2
47	2p	80	PHE	2.2
1	1A	899	A	2.2
1	2A	652(A)	A	2.2
1	2A	896	A	2.2
8	1I	35	LEU	2.2
10	2O	91	LEU	2.2
54	2w	15	A	2.2
54	2w	46	A	2.2
38	2g	113	GLU	2.2
7	2H	134	SER	2.2
26	24	46	GLN	2.1
38	2g	97	GLN	2.1
6	2G	25	TYR	2.1
1	1A	2153	G	2.1
21	2Z	165	VAL	2.1
32	2a	1120	G	2.1
33	1b	165	VAL	2.1
44	2m	5	ALA	2.1
14	2S	30	ARG	2.1
29	27	23	ARG	2.1
44	2m	49	THR	2.1
18	2W	14	PRO	2.1
32	1a	1019	C	2.1
34	1c	10	PHE	2.1
38	2g	62	PHE	2.1
40	2i	101	PHE	2.1
14	2S	26	LEU	2.1
21	2Z	67	LEU	2.1
40	1i	50	LEU	2.1
44	1m	96	LEU	2.1
31	29	8	LYS	2.1
7	2H	86	GLU	2.1
35	1d	156	GLU	2.1
40	2i	80	GLY	2.1
7	2H	112	PRO	2.1
26	24	5	ILE	2.1
40	2i	70	LYS	2.1
48	2q	65	ILE	2.1
54	1w	51	G	2.1
7	2H	98	LEU	2.1
16	1U	117	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
39	2h	63	LEU	2.1
48	2q	74	LEU	2.1
54	2w	62	C	2.1
21	1Z	151	HIS	2.1
34	2c	20	SER	2.1
32	2a	1287	A	2.1
33	2b	209	ARG	2.1
50	1s	36	ARG	2.1
53	1v	23	A	2.1
34	1c	81	GLY	2.1
5	2F	73	ALA	2.1
14	2S	100	ALA	2.1
17	2V	5	VAL	2.1
21	2Z	86	VAL	2.1
32	2a	1358	U	2.1
40	1i	27	THR	2.1
52	2u	17	THR	2.1
8	1I	132	PRO	2.1
16	2U	2	PRO	2.1
34	2c	28	GLN	2.1
42	1k	29	ILE	2.1
47	2p	48	TRP	2.1
33	1b	11	LEU	2.1
39	1h	112	LEU	2.1
40	1i	102	LEU	2.1
47	2p	74	LEU	2.1
1	1A	2155	G	2.1
31	29	9	ARG	2.1
32	1a	1274	G	2.1
33	2b	170	GLU	2.1
33	2b	210	SER	2.1
48	2q	12	SER	2.1
40	2i	23	ASN	2.1
36	1e	10	MET	2.1
3	2D	126	GLN	2.1
12	2Q	113	GLN	2.1
31	19	16	VAL	2.1
38	1g	108	ALA	2.1
34	2c	191	THR	2.1
35	2d	4	TYR	2.1
45	2n	18	VAL	2.1
48	2q	11	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
51	1t	88	VAL	2.1
6	2G	161	THR	2.1
7	2H	162	ILE	2.1
45	2n	7	ILE	2.1
8	2I	72	LEU	2.1
17	2V	21	ARG	2.1
35	2d	115	ARG	2.1
36	2e	28	PHE	2.1
34	2c	56	ASP	2.1
32	1a	68	G	2.1
32	1a	163	C	2.1
32	1a	1017	G	2.1
3	2D	51	VAL	2.1
6	2G	73	ALA	2.1
20	2Y	65	ALA	2.1
38	2g	121	ALA	2.1
45	1n	48	ALA	2.1
47	1p	2	VAL	2.1
50	2s	75	ALA	2.1
26	24	11	PRO	2.1
32	2a	1012	U	2.1
32	2a	1357	A	2.1
36	2e	49	PRO	2.1
54	2w	41	U	2.1
6	2G	95	ARG	2.1
41	1j	46	ARG	2.1
41	2j	60	ARG	2.1
6	1G	63	ILE	2.1
6	1G	157	ILE	2.1
6	2G	63	ILE	2.1
16	2U	62	ILE	2.1
21	2Z	53	ILE	2.1
36	2e	101	ILE	2.1
4	2E	5	LEU	2.1
14	2S	31	SER	2.1
33	2b	19	HIS	2.1
41	2j	12	ASP	2.1
35	2d	196	LEU	2.1
32	1a	1043	C	2.1
32	1a	1158	C	2.1
36	1e	81	GLU	2.1
41	2j	25	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	2A	2101	G	2.1
23	21	69	LYS	2.1
33	1b	137	ARG	2.1
38	2g	10	ARG	2.1
38	2g	147	ALA	2.1
20	2Y	42	VAL	2.1
41	2j	73	ASP	2.1
1	1A	887	A	2.1
8	2I	79	ILE	2.1
50	1s	49	ILE	2.1
50	1s	57	HIS	2.1
4	2E	96	PHE	2.1
8	2I	77	LEU	2.1
33	2b	233	SER	2.1
35	2d	79	PHE	2.1
36	2e	110	LEU	2.1
37	1f	21	LEU	2.1
42	2k	90	GLY	2.1
45	2n	24	CYS	2.1
50	2s	26	GLY	2.1
38	2g	103	TRP	2.1
14	2S	20	ARG	2.1
33	2b	144	ARG	2.1
34	1c	172	ARG	2.1
34	1c	190	ARG	2.1
40	1i	51	ARG	2.1
29	17	1	MET	2.0
6	2G	17	PRO	2.0
16	1U	4	ALA	2.0
32	2a	91	C	2.0
32	2a	1060	C	2.0
33	1b	207	ALA	2.0
40	1i	105	ASP	2.0
48	1q	28	PRO	2.0
1	1A	2189	U	2.0
3	1D	51	VAL	2.0
5	2F	183	VAL	2.0
14	2S	49	VAL	2.0
17	2V	79	VAL	2.0
46	2o	25	THR	2.0
54	2w	65	U	2.0
57	2y	59	U	2.0

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Mol	Chain	Res	Type	RSRZ
1	1A	1089	G	2.0
1	2A	2124	G	2.0
1	2A	899	A	2.0
11	2P	144	GLU	2.0
31	29	17	ILE	2.0
34	2c	89	GLU	2.0
50	1s	22	LEU	2.0
3	2D	251	GLY	2.0
35	1d	16	GLY	2.0
39	2h	128	GLY	2.0
6	2G	182	LYS	2.0
26	14	58	ARG	2.0
5	2F	80	ALA	2.0
11	2P	134	ALA	2.0
49	1r	73	ALA	2.0
15	2T	30	VAL	2.0
17	2V	14	VAL	2.0
32	1a	848	C	2.0
32	2a	1122	U	2.0
44	2m	73	GLU	2.0
57	1y	69	C	2.0
4	2E	52	LEU	2.0
12	2Q	64	ILE	2.0
25	23	15	TYR	2.0
35	2d	69	GLY	2.0
38	1g	120	ILE	2.0
38	2g	101	LEU	2.0
45	2n	28	GLY	2.0
41	1j	66	ARG	2.0
1	1A	1055	G	2.0
1	2A	882	G	2.0
32	2a	1133	G	2.0
32	2a	1447	A	2.0
34	1c	56	ASP	2.0
33	1b	129	GLU	2.0
7	2H	146	ALA	2.0
33	1b	24	TRP	2.0
33	2b	188	ALA	2.0
40	1i	84	ALA	2.0
4	2E	105	THR	2.0
33	2b	103	THR	2.0
40	2i	97	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
45	2n	27	CYS	2.0
7	2H	114	VAL	2.0
8	1I	74	ASN	2.0
18	2W	20	VAL	2.0
54	1w	60	U	2.0
3	1D	176	ARG	2.0
11	2P	116	GLY	2.0
21	1Z	122	ARG	2.0
34	2c	194	GLY	2.0
36	2e	22	GLY	2.0
38	1g	130	GLY	2.0
43	1l	63	GLY	2.0
5	2F	12	LEU	2.0
8	2I	6	LEU	2.0
16	2U	98	LEU	2.0
25	23	23	LEU	2.0
33	2b	154	LEU	2.0
34	1c	134	ILE	2.0
54	2w	48	C	2.0
35	2d	135	LEU	2.0
46	2o	32	LEU	2.0
50	2s	61	TYR	2.0
1	1A	2207	G	2.0
1	2A	1169	G	2.0
1	2A	2119	A	2.0
32	2a	1117	G	2.0
32	2a	1258	G	2.0
51	1t	29	LYS	2.0
34	2c	37	GLN	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	5MU	2y	54	21/22	0.57	0.53	101,111,118,134	0
57	4SU	2y	8	20/21	0.60	0.26	105,113,122,131	0
54	4SU	2w	8	20/21	0.66	0.30	104,111,124,129	0
57	PSU	1y	55	20/21	0.68	0.52	104,112,117,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	4SU	1y	8	20/21	0.72	0.36	105,110,118,129	0
54	4SU	1w	8	20/21	0.75	0.29	102,109,124,127	0
57	5MU	1y	54	21/22	0.76	0.54	105,110,115,127	0
54	5MU	2w	54	21/22	0.76	0.22	100,104,109,115	0
54	PSU	1w	55	20/21	0.76	0.38	97,100,112,112	0
57	PSU	2y	55	20/21	0.77	0.48	107,112,118,123	0
54	PSU	2w	55	20/21	0.78	0.32	104,108,117,120	0
54	5MU	1w	54	21/22	0.82	0.25	78,95,98,101	0
32	2MG	2a	1207	24/25	0.85	0.16	91,96,103,113	0
1	5MU	2A	1915	21/22	0.88	0.20	80,89,91,95	0
55	4SU	2x	8	20/21	0.88	0.18	91,96,99,103	0
43	0TD	1l	92	10/11	0.90	0.23	66,75,78,95	0
32	PSU	2a	516	20/21	0.91	0.16	80,89,93,95	0
55	5MU	2x	54	21/22	0.91	0.17	89,96,98,104	0
55	PSU	1x	55	20/21	0.91	0.14	66,77,86,93	0
55	PSU	2x	55	20/21	0.91	0.12	86,92,99,102	0
1	5MU	1A	1915	21/22	0.91	0.19	64,74,80,81	0
43	0TD	2l	92	10/11	0.92	0.19	78,82,86,87	0
32	5MC	2a	967	21/22	0.93	0.15	75,80,88,98	0
54	L3X	2w	76	26/27	0.93	0.27	63,71,76,83	0
32	M2G	2a	966	25/26	0.93	0.19	67,79,96,97	0
56	FME	2z	1	10/11	0.93	0.40	66,76,86,87	0
55	5MU	1x	54	21/22	0.93	0.15	74,81,89,91	0
32	G7M	2a	527	24/25	0.94	0.17	75,82,88,93	0
32	2MG	1a	1207	24/25	0.94	0.12	81,85,89,95	0
1	PSU	2A	1917	20/21	0.94	0.18	74,83,87,88	0
56	FME	1z	1	10/11	0.94	0.38	50,57,73,78	0
1	OMC	2A	1920	21/22	0.94	0.21	65,73,78,80	0
32	5MC	2a	1400	21/22	0.94	0.20	81,85,89,91	0
32	5MC	2a	1404	21/22	0.94	0.20	60,71,76,79	0
32	5MC	2a	1407	21/22	0.94	0.20	61,68,74,77	0
32	MA6	2a	1519	24/25	0.94	0.23	63,77,83,84	0
55	5MC	2x	32	21/22	0.94	0.15	79,85,90,95	0
1	PSU	2A	1911	20/21	0.94	0.19	72,75,80,80	0
55	8AN	2x	76	22/23	0.95	0.24	55,65,72,76	0
55	4SU	1x	8	20/21	0.95	0.18	64,71,75,80	0
32	UR3	2a	1498	21/22	0.95	0.22	63,69,77,78	0
55	5MC	1x	32	21/22	0.95	0.18	62,68,72,78	0
32	5MC	1a	967	21/22	0.95	0.15	58,64,71,78	0
32	4OC	2a	1402	22/23	0.95	0.19	68,76,80,81	0
1	PSU	1A	1917	20/21	0.95	0.17	59,68,76,76	0
54	L3X	1w	76	26/27	0.95	0.19	42,52,59,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	PSU	1a	516	20/21	0.95	0.14	72,77,81,81	0
32	MA6	2a	1518	24/25	0.96	0.21	64,79,83,84	0
1	5MC	2A	1962	21/22	0.96	0.25	43,57,66,73	0
1	OMU	2A	2552	21/22	0.96	0.22	47,55,61,64	0
32	M2G	1a	966	25/26	0.96	0.16	58,63,72,80	0
32	5MC	1a	1407	21/22	0.97	0.21	44,52,56,59	0
1	PSU	1A	1911	20/21	0.97	0.18	51,59,64,65	0
55	8AN	1x	76	22/23	0.97	0.20	35,46,52,62	0
1	PSU	2A	2605	20/21	0.97	0.21	40,49,59,59	0
1	5MC	1A	1942	21/22	0.97	0.22	42,47,52,61	0
1	5MC	2A	1942	21/22	0.97	0.21	58,69,73,79	0
1	2MA	2A	2503	23/24	0.98	0.23	43,48,51,53	0
32	5MC	1a	1404	21/22	0.98	0.19	46,52,55,58	0
1	PSU	1A	2605	20/21	0.98	0.21	33,37,45,46	0
32	MA6	1a	1518	24/25	0.98	0.22	46,52,55,58	0
32	MA6	1a	1519	24/25	0.98	0.23	45,55,58,61	0
1	5MU	1A	1939	21/22	0.98	0.22	31,36,41,43	0
32	G7M	1a	527	24/25	0.98	0.16	62,68,71,74	0
1	OMC	1A	1920	21/22	0.98	0.21	45,54,59,63	0
1	5MC	1A	1962	21/22	0.98	0.20	40,43,48,56	0
1	OMG	1A	2251	24/25	0.98	0.22	26,33,37,41	0
1	5MU	2A	1939	21/22	0.98	0.22	42,50,56,58	0
32	5MC	1a	1400	21/22	0.98	0.16	56,65,67,70	0
32	4OC	1a	1402	22/23	0.98	0.21	47,56,61,67	0
1	OMG	2A	2251	24/25	0.98	0.21	47,52,58,64	0
32	UR3	1a	1498	21/22	0.99	0.21	46,52,57,61	0
1	2MA	1A	2503	23/24	0.99	0.21	24,31,33,35	0
1	OMU	1A	2552	21/22	0.99	0.21	30,37,40,41	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	1A	3965	1/1	0.12	0.12	75,75,75,75	0
58	MG	1w	106	1/1	0.28	0.30	97,97,97,97	0
58	MG	2A	3281	1/1	0.31	0.38	89,89,89,89	0
58	MG	2a	1606	1/1	0.32	0.12	86,86,86,86	0
58	MG	1A	3524	1/1	0.41	0.47	72,72,72,72	0
58	MG	2A	3051	1/1	0.41	0.58	90,90,90,90	0
58	MG	2A	3346	1/1	0.43	0.17	80,80,80,80	0
58	MG	1A	4018	1/1	0.43	0.16	72,72,72,72	0
58	MG	2B	210	1/1	0.44	0.17	92,92,92,92	0
58	MG	1A	4037	1/1	0.44	0.15	55,55,55,55	0
58	MG	1a	1605	1/1	0.45	0.20	78,78,78,78	0
58	MG	2w	102	1/1	0.45	0.29	92,92,92,92	0
58	MG	2A	3413	1/1	0.48	0.41	78,78,78,78	0
58	MG	2A	3134	1/1	0.48	0.15	78,78,78,78	0
58	MG	1A	3254	1/1	0.49	0.44	75,75,75,75	0
58	MG	2A	3251	1/1	0.50	0.22	77,77,77,77	0
58	MG	1a	1771	1/1	0.50	0.30	97,97,97,97	0
58	MG	2A	3538	1/1	0.50	0.09	81,81,81,81	0
58	MG	1A	4051	1/1	0.51	0.45	78,78,78,78	0
58	MG	2A	3342	1/1	0.51	0.18	73,73,73,73	0
58	MG	1A	4023	1/1	0.52	0.11	96,96,96,96	0
58	MG	1A	3792	1/1	0.53	0.29	59,59,59,59	0
58	MG	1w	102	1/1	0.53	0.27	93,93,93,93	0
58	MG	2Q	203	1/1	0.54	0.36	72,72,72,72	0
58	MG	2A	3307	1/1	0.54	0.33	78,78,78,78	0
58	MG	2A	3067	1/1	0.54	0.12	75,75,75,75	0
58	MG	2A	3769	1/1	0.55	0.26	49,49,49,49	0
58	MG	1w	101	1/1	0.56	0.16	97,97,97,97	0
58	MG	1a	1607	1/1	0.56	0.26	80,80,80,80	0
58	MG	2g	201	1/1	0.56	0.16	89,89,89,89	0
58	MG	2A	3201	1/1	0.56	0.19	86,86,86,86	0
58	MG	1A	3469	1/1	0.57	0.19	72,72,72,72	0
58	MG	1a	1727	1/1	0.57	0.27	90,90,90,90	0
58	MG	2A	3005	1/1	0.57	0.17	75,75,75,75	0
58	MG	2A	3654	1/1	0.57	0.19	79,79,79,79	0
58	MG	2A	3008	1/1	0.57	0.37	70,70,70,70	0
58	MG	1B	234	1/1	0.58	0.15	80,80,80,80	0
58	MG	1A	3489	1/1	0.58	0.41	77,77,77,77	0
58	MG	2a	1802	1/1	0.59	0.17	76,76,76,76	0
58	MG	2A	3599	1/1	0.59	0.23	73,73,73,73	0
58	MG	2A	3335	1/1	0.59	0.28	74,74,74,74	0
58	MG	2A	3121	1/1	0.60	0.18	68,68,68,68	0
58	MG	1A	3478	1/1	0.60	0.12	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3317	1/1	0.60	0.19	47,47,47,47	0
58	MG	2a	1820	1/1	0.60	0.21	80,80,80,80	0
58	MG	1a	1630	1/1	0.60	0.20	75,75,75,75	0
58	MG	18	106	1/1	0.60	0.34	76,76,76,76	0
58	MG	2A	3063	1/1	0.61	0.38	66,66,66,66	0
58	MG	2A	3239	1/1	0.61	0.25	65,65,65,65	0
58	MG	1A	3984	1/1	0.61	0.16	68,68,68,68	0
58	MG	2a	1706	1/1	0.61	0.10	89,89,89,89	0
58	MG	1A	3208	1/1	0.61	0.14	81,81,81,81	0
58	MG	1A	3365	1/1	0.61	0.43	60,60,60,60	0
58	MG	2A	3319	1/1	0.61	0.92	70,70,70,70	0
58	MG	2A	3189	1/1	0.61	0.26	76,76,76,76	0
58	MG	2A	3316	1/1	0.62	0.20	81,81,81,81	0
58	MG	1A	3231	1/1	0.62	0.25	76,76,76,76	0
58	MG	1A	3410	1/1	0.62	0.23	93,93,93,93	0
58	MG	2A	3589	1/1	0.62	0.13	72,72,72,72	0
58	MG	2A	3184	1/1	0.62	0.35	83,83,83,83	0
58	MG	2A	3261	1/1	0.63	0.30	73,73,73,73	0
58	MG	2A	3532	1/1	0.63	0.21	51,51,51,51	0
58	MG	1A	3587	1/1	0.63	0.14	60,60,60,60	0
58	MG	2A	3682	1/1	0.63	0.26	75,75,75,75	0
58	MG	2a	1625	1/1	0.63	0.36	73,73,73,73	0
58	MG	1A	3783	1/1	0.64	0.12	64,64,64,64	0
58	MG	2A	3255	1/1	0.64	0.29	85,85,85,85	0
58	MG	1a	1645	1/1	0.64	0.17	77,77,77,77	0
58	MG	2a	1624	1/1	0.64	0.30	83,83,83,83	0
58	MG	1a	1676	1/1	0.64	0.25	85,85,85,85	0
58	MG	1A	3423	1/1	0.64	0.29	64,64,64,64	0
58	MG	2a	1795	1/1	0.64	0.21	93,93,93,93	0
58	MG	1A	3387	1/1	0.64	0.21	67,67,67,67	0
58	MG	2A	3194	1/1	0.64	0.41	89,89,89,89	0
58	MG	2A	3055	1/1	0.64	0.18	70,70,70,70	0
58	MG	1A	3371	1/1	0.64	0.43	58,58,58,58	0
58	MG	1x	103	1/1	0.65	0.42	87,87,87,87	0
58	MG	1a	1714	1/1	0.65	0.36	75,75,75,75	0
58	MG	1A	3299	1/1	0.65	0.21	65,65,65,65	0
58	MG	1a	1757	1/1	0.65	0.22	79,79,79,79	0
58	MG	1A	3514	1/1	0.65	0.32	67,67,67,67	0
58	MG	1A	3460	1/1	0.65	0.22	59,59,59,59	0
58	MG	1A	3584	1/1	0.65	0.21	53,53,53,53	0
58	MG	2A	3716	1/1	0.65	0.14	90,90,90,90	0
58	MG	1A	3480	1/1	0.65	0.55	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	2A	3373	1/1	0.65	0.19	86,86,86,86	0
58	MG	2B	205	1/1	0.66	0.18	79,79,79,79	0
58	MG	1A	4058	1/1	0.66	0.14	69,69,69,69	0
58	MG	2E	307	1/1	0.66	0.21	75,75,75,75	0
58	MG	2A	3266	1/1	0.66	0.32	83,83,83,83	0
58	MG	1A	3431	1/1	0.66	0.23	65,65,65,65	0
58	MG	1A	3884	1/1	0.66	0.12	74,74,74,74	0
58	MG	2A	3580	1/1	0.66	0.12	75,75,75,75	0
58	MG	1A	3353	1/1	0.66	0.24	69,69,69,69	0
58	MG	1A	3539	1/1	0.66	0.37	59,59,59,59	0
58	MG	2A	3102	1/1	0.66	0.26	86,86,86,86	0
58	MG	2A	3341	1/1	0.66	0.15	79,79,79,79	0
58	MG	1a	1622	1/1	0.66	0.17	83,83,83,83	0
58	MG	2A	3132	1/1	0.66	0.24	69,69,69,69	0
58	MG	2A	3193	1/1	0.67	0.27	79,79,79,79	0
58	MG	1F	311	1/1	0.67	0.24	63,63,63,63	0
58	MG	1A	3830	1/1	0.67	0.17	70,70,70,70	0
58	MG	1A	3948	1/1	0.67	0.12	40,40,40,40	0
58	MG	2a	1761	1/1	0.67	0.17	86,86,86,86	0
58	MG	1a	1712	1/1	0.67	0.28	74,74,74,74	0
58	MG	1A	4075	1/1	0.67	0.17	91,91,91,91	0
58	MG	2A	3562	1/1	0.67	0.38	71,71,71,71	0
58	MG	2A	3337	1/1	0.67	0.32	73,73,73,73	0
58	MG	1A	3999	1/1	0.67	0.09	83,83,83,83	0
58	MG	1w	105	1/1	0.68	0.16	84,84,84,84	0
58	MG	2A	3140	1/1	0.68	0.25	81,81,81,81	0
58	MG	2A	3718	1/1	0.68	0.15	52,52,52,52	0
58	MG	2A	3737	1/1	0.68	0.12	82,82,82,82	0
58	MG	2a	1709	1/1	0.68	0.13	90,90,90,90	0
58	MG	2A	3073	1/1	0.68	0.20	62,62,62,62	0
58	MG	2a	1779	1/1	0.68	0.14	95,95,95,95	0
58	MG	1A	3057	1/1	0.68	0.19	60,60,60,60	0
58	MG	1A	3560	1/1	0.68	0.18	63,63,63,63	0
58	MG	1A	3691	1/1	0.68	0.18	56,56,56,56	0
58	MG	2A	3681	1/1	0.68	0.10	81,81,81,81	0
58	MG	2R	202	1/1	0.68	0.19	75,75,75,75	0
58	MG	2A	3756	1/1	0.69	0.08	92,92,92,92	0
58	MG	2a	1638	1/1	0.69	0.13	76,76,76,76	0
58	MG	2A	3609	1/1	0.69	0.15	74,74,74,74	0
58	MG	2A	3219	1/1	0.69	0.56	73,73,73,73	0
58	MG	1A	3981	1/1	0.69	0.13	84,84,84,84	0
58	MG	1A	3327	1/1	0.69	0.23	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3352	1/1	0.69	0.38	60,60,60,60	0
58	MG	2A	3336	1/1	0.69	0.32	76,76,76,76	0
58	MG	2T	202	1/1	0.69	0.23	81,81,81,81	0
58	MG	1A	3263	1/1	0.69	0.25	77,77,77,77	0
58	MG	2q	202	1/1	0.69	0.08	92,92,92,92	0
58	MG	2A	3743	1/1	0.69	0.24	61,61,61,61	0
58	MG	2a	1613	1/1	0.70	0.15	79,79,79,79	0
58	MG	1w	108	1/1	0.70	0.19	87,87,87,87	0
58	MG	1a	1637	1/1	0.70	0.35	82,82,82,82	0
58	MG	1A	3128	1/1	0.70	0.17	61,61,61,61	0
58	MG	2a	1678	1/1	0.70	0.09	70,70,70,70	0
58	MG	1a	1675	1/1	0.70	0.18	67,67,67,67	0
58	MG	1A	4021	1/1	0.70	0.06	65,65,65,65	0
58	MG	2A	3652	1/1	0.70	0.14	75,75,75,75	0
58	MG	1a	1705	1/1	0.70	0.24	89,89,89,89	0
58	MG	2A	3678	1/1	0.70	0.16	62,62,62,62	0
58	MG	2a	1801	1/1	0.70	0.20	76,76,76,76	0
58	MG	1A	3572	1/1	0.70	0.15	81,81,81,81	0
58	MG	1A	4060	1/1	0.70	0.35	49,49,49,49	0
58	MG	2A	3693	1/1	0.70	0.55	64,64,64,64	0
58	MG	2a	1602	1/1	0.70	0.18	81,81,81,81	0
58	MG	2A	3546	1/1	0.70	0.10	91,91,91,91	0
58	MG	2x	106	1/1	0.70	0.09	81,81,81,81	0
58	MG	1A	3913	1/1	0.71	0.09	75,75,75,75	0
58	MG	2a	1666	1/1	0.71	0.49	87,87,87,87	0
58	MG	1A	3336	1/1	0.71	0.15	59,59,59,59	0
58	MG	1A	3073	1/1	0.71	0.33	67,67,67,67	0
58	MG	1A	3521	1/1	0.71	0.43	81,81,81,81	0
58	MG	2A	3190	1/1	0.71	0.50	85,85,85,85	0
58	MG	2A	3083	1/1	0.71	0.29	64,64,64,64	0
58	MG	2A	3288	1/1	0.71	0.35	72,72,72,72	0
58	MG	1A	4041	1/1	0.71	0.20	59,59,59,59	0
58	MG	2Z	301	1/1	0.71	0.36	97,97,97,97	0
58	MG	1A	3122	1/1	0.71	0.26	58,58,58,58	0
58	MG	2A	3207	1/1	0.71	0.41	74,74,74,74	0
58	MG	1A	3535	1/1	0.71	0.30	76,76,76,76	0
58	MG	2A	3564	1/1	0.71	0.32	65,65,65,65	0
58	MG	2A	3232	1/1	0.71	0.37	84,84,84,84	0
58	MG	2A	3405	1/1	0.72	0.29	85,85,85,85	0
58	MG	2a	1658	1/1	0.72	0.15	79,79,79,79	0
58	MG	2A	3787	1/1	0.72	0.37	79,79,79,79	0
58	MG	2A	3801	1/1	0.72	0.35	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3643	1/1	0.72	0.16	69,69,69,69	0
58	MG	1A	3531	1/1	0.72	0.28	71,71,71,71	0
58	MG	2A	3420	1/1	0.72	0.14	60,60,60,60	0
58	MG	1A	3582	1/1	0.72	0.14	79,79,79,79	0
58	MG	2A	3533	1/1	0.72	0.21	68,68,68,68	0
58	MG	2A	3080	1/1	0.72	0.47	67,67,67,67	0
58	MG	1a	1747	1/1	0.72	0.18	80,80,80,80	0
58	MG	1A	3261	1/1	0.72	0.10	77,77,77,77	0
58	MG	1A	3865	1/1	0.72	0.11	50,50,50,50	0
58	MG	1A	3461	1/1	0.72	0.34	81,81,81,81	0
58	MG	1A	4001	1/1	0.72	0.13	62,62,62,62	0
58	MG	1A	3412	1/1	0.72	0.58	65,65,65,65	0
58	MG	26	101	1/1	0.73	0.22	76,76,76,76	0
58	MG	2A	3034	1/1	0.73	0.19	78,78,78,78	0
58	MG	2A	3042	1/1	0.73	0.25	71,71,71,71	0
58	MG	1A	3356	1/1	0.73	0.14	67,67,67,67	0
58	MG	1A	3362	1/1	0.73	0.18	58,58,58,58	0
58	MG	2A	3688	1/1	0.73	0.17	74,74,74,74	0
58	MG	1A	3809	1/1	0.73	0.23	61,61,61,61	0
58	MG	1A	3988	1/1	0.73	0.23	78,78,78,78	0
58	MG	1A	3004	1/1	0.73	0.20	33,33,33,33	0
58	MG	1A	3369	1/1	0.73	0.52	58,58,58,58	0
58	MG	1w	104	1/1	0.73	0.17	81,81,81,81	0
58	MG	1A	3259	1/1	0.73	0.32	62,62,62,62	0
58	MG	2a	1712	1/1	0.73	0.31	84,84,84,84	0
58	MG	2A	3111	1/1	0.73	0.21	75,75,75,75	0
58	MG	2A	3112	1/1	0.73	0.19	84,84,84,84	0
58	MG	2A	3114	1/1	0.73	0.24	60,60,60,60	0
58	MG	1E	308	1/1	0.73	0.28	67,67,67,67	0
58	MG	1A	3352	1/1	0.73	0.44	80,80,80,80	0
58	MG	1x	101	1/1	0.73	1.15	98,98,98,98	0
58	MG	1a	1710	1/1	0.73	0.15	70,70,70,70	0
58	MG	2A	3168	1/1	0.73	0.18	77,77,77,77	0
58	MG	1G	204	1/1	0.73	0.08	84,84,84,84	0
58	MG	1A	3144	1/1	0.73	0.21	51,51,51,51	0
58	MG	1A	3758	1/1	0.74	0.09	72,72,72,72	0
58	MG	2B	211	1/1	0.74	0.12	86,86,86,86	0
58	MG	2B	216	1/1	0.74	0.10	83,83,83,83	0
58	MG	2a	1690	1/1	0.74	0.21	95,95,95,95	0
58	MG	2A	3365	1/1	0.74	0.42	66,66,66,66	0
58	MG	1A	3354	1/1	0.74	0.17	63,63,63,63	0
58	MG	2A	3388	1/1	0.74	0.29	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2a	1722	1/1	0.74	0.23	85,85,85,85	0
58	MG	2A	3393	1/1	0.74	0.37	84,84,84,84	0
58	MG	1A	3002	1/1	0.74	0.20	53,53,53,53	0
58	MG	1A	3024	1/1	0.74	0.24	75,75,75,75	0
58	MG	1A	3541	1/1	0.74	0.28	72,72,72,72	0
58	MG	2A	3465	1/1	0.74	0.14	53,53,53,53	0
58	MG	2A	3784	1/1	0.74	0.26	90,90,90,90	0
58	MG	2a	1621	1/1	0.74	0.23	81,81,81,81	0
58	MG	2A	3098	1/1	0.74	0.18	88,88,88,88	0
58	MG	1A	3082	1/1	0.74	0.36	53,53,53,53	0
58	MG	1B	203	1/1	0.74	0.16	52,52,52,52	0
58	MG	1A	3143	1/1	0.75	0.19	54,54,54,54	0
58	MG	1S	203	1/1	0.75	0.18	66,66,66,66	0
58	MG	2A	3343	1/1	0.75	0.13	83,83,83,83	0
58	MG	2a	1702	1/1	0.75	0.35	76,76,76,76	0
58	MG	2A	3020	1/1	0.75	0.18	76,76,76,76	0
58	MG	2A	3279	1/1	0.75	0.24	74,74,74,74	0
58	MG	1A	4067	1/1	0.75	0.10	52,52,52,52	0
58	MG	1w	103	1/1	0.75	0.14	71,71,71,71	0
58	MG	1A	3664	1/1	0.75	0.15	73,73,73,73	0
58	MG	1A	4039	1/1	0.75	0.28	72,72,72,72	0
58	MG	1A	3148	1/1	0.75	0.55	56,56,56,56	0
58	MG	2a	1619	1/1	0.75	0.21	80,80,80,80	0
58	MG	2A	3328	1/1	0.75	0.23	68,68,68,68	0
58	MG	1D	3604	1/1	0.75	0.19	54,54,54,54	0
58	MG	2A	3672	1/1	0.75	0.29	52,52,52,52	0
58	MG	2a	1631	1/1	0.75	0.52	74,74,74,74	0
58	MG	1A	3436	1/1	0.75	0.54	60,60,60,60	0
58	MG	1A	3191	1/1	0.75	0.12	66,66,66,66	0
58	MG	2A	3332	1/1	0.76	0.25	74,74,74,74	0
58	MG	1A	3449	1/1	0.76	0.20	78,78,78,78	0
58	MG	1A	3409	1/1	0.76	0.20	65,65,65,65	0
58	MG	2A	3749	1/1	0.76	0.17	76,76,76,76	0
58	MG	2a	1634	1/1	0.76	0.14	86,86,86,86	0
58	MG	1a	1633	1/1	0.76	0.24	88,88,88,88	0
58	MG	1A	3213	1/1	0.76	0.15	59,59,59,59	0
58	MG	2A	3575	1/1	0.76	0.12	66,66,66,66	0
58	MG	1m	3001	1/1	0.76	0.07	75,75,75,75	0
58	MG	2A	3585	1/1	0.76	0.18	73,73,73,73	0
58	MG	1A	3232	1/1	0.76	0.32	65,65,65,65	0
58	MG	1a	1668	1/1	0.76	0.18	73,73,73,73	0
58	MG	2A	3264	1/1	0.76	0.18	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3622	1/1	0.76	0.16	81,81,81,81	0
58	MG	2A	3150	1/1	0.76	0.24	69,69,69,69	0
58	MG	2a	1733	1/1	0.76	0.10	95,95,95,95	0
58	MG	2a	1751	1/1	0.76	0.19	88,88,88,88	0
58	MG	2G	201	1/1	0.76	0.12	81,81,81,81	0
58	MG	2A	3267	1/1	0.76	0.26	89,89,89,89	0
58	MG	1A	3360	1/1	0.76	0.19	67,67,67,67	0
58	MG	1A	4066	1/1	0.76	0.15	49,49,49,49	0
58	MG	2A	3400	1/1	0.76	0.13	77,77,77,77	0
58	MG	18	103	1/1	0.76	0.24	59,59,59,59	0
58	MG	1A	3293	1/1	0.76	0.18	56,56,56,56	0
58	MG	1A	3395	1/1	0.76	0.42	67,67,67,67	0
58	MG	1a	1713	1/1	0.76	0.21	67,67,67,67	0
58	MG	1A	3448	1/1	0.76	0.40	49,49,49,49	0
58	MG	1a	1664	1/1	0.77	0.21	80,80,80,80	0
58	MG	1A	3473	1/1	0.77	0.18	55,55,55,55	0
58	MG	1a	1742	1/1	0.77	0.21	70,70,70,70	0
58	MG	2A	3608	1/1	0.77	0.24	70,70,70,70	0
58	MG	1A	3726	1/1	0.77	0.20	45,45,45,45	0
58	MG	2A	3395	1/1	0.77	0.40	73,73,73,73	0
58	MG	1A	3837	1/1	0.77	0.09	78,78,78,78	0
58	MG	2A	3229	1/1	0.77	0.36	70,70,70,70	0
58	MG	2A	3327	1/1	0.77	0.33	77,77,77,77	0
58	MG	2A	3137	1/1	0.77	0.41	67,67,67,67	0
58	MG	1a	1684	1/1	0.77	0.39	63,63,63,63	0
58	MG	2A	3481	1/1	0.77	0.22	48,48,48,48	0
58	MG	2A	3242	1/1	0.77	0.19	71,71,71,71	0
58	MG	1A	3530	1/1	0.77	0.20	57,57,57,57	0
58	MG	2a	1754	1/1	0.77	0.17	75,75,75,75	0
58	MG	20	101	1/1	0.77	0.41	81,81,81,81	0
58	MG	2A	3166	1/1	0.77	0.14	87,87,87,87	0
58	MG	2a	1601	1/1	0.77	0.09	87,87,87,87	0
58	MG	2A	3257	1/1	0.77	0.21	82,82,82,82	0
58	MG	1A	3245	1/1	0.77	0.55	60,60,60,60	0
58	MG	1A	3907	1/1	0.77	0.11	81,81,81,81	0
58	MG	2A	3030	1/1	0.77	0.19	69,69,69,69	0
58	MG	2A	3746	1/1	0.77	0.23	71,71,71,71	0
58	MG	1A	3025	1/1	0.77	0.28	42,42,42,42	0
58	MG	2A	3581	1/1	0.77	0.26	79,79,79,79	0
58	MG	1A	3866	1/1	0.78	0.17	53,53,53,53	0
58	MG	2A	3407	1/1	0.78	0.33	75,75,75,75	0
58	MG	2A	3284	1/1	0.78	0.76	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	3687	1/1	0.78	0.21	68,68,68,68	0
58	MG	2A	3285	1/1	0.78	0.36	68,68,68,68	0
58	MG	2A	3451	1/1	0.78	0.26	66,66,66,66	0
58	MG	1A	3403	1/1	0.78	0.17	61,61,61,61	0
58	MG	1A	3885	1/1	0.78	0.20	63,63,63,63	0
58	MG	2a	1633	1/1	0.78	0.24	86,86,86,86	0
58	MG	2A	3498	1/1	0.78	0.12	84,84,84,84	0
58	MG	2a	1637	1/1	0.78	0.36	76,76,76,76	0
58	MG	1B	202	1/1	0.78	0.38	64,64,64,64	0
58	MG	2a	1650	1/1	0.78	0.10	95,95,95,95	0
58	MG	2a	1657	1/1	0.78	0.12	88,88,88,88	0
58	MG	2A	3199	1/1	0.78	0.20	76,76,76,76	0
58	MG	1A	3760	1/1	0.78	0.19	43,43,43,43	0
58	MG	2A	3204	1/1	0.78	0.48	58,58,58,58	0
58	MG	2A	3206	1/1	0.78	0.15	79,79,79,79	0
58	MG	1B	209	1/1	0.78	0.27	56,56,56,56	0
58	MG	2a	1705	1/1	0.78	0.06	90,90,90,90	0
58	MG	1B	228	1/1	0.78	0.15	87,87,87,87	0
58	MG	2a	1708	1/1	0.78	0.06	82,82,82,82	0
58	MG	2A	3794	1/1	0.78	0.11	74,74,74,74	0
58	MG	2a	1711	1/1	0.78	0.39	91,91,91,91	0
58	MG	2A	3576	1/1	0.78	0.11	69,69,69,69	0
58	MG	2A	3018	1/1	0.78	0.16	66,66,66,66	0
58	MG	1A	3099	1/1	0.78	0.14	68,68,68,68	0
58	MG	2A	3122	1/1	0.78	0.12	62,62,62,62	0
58	MG	2A	3586	1/1	0.78	0.22	82,82,82,82	0
58	MG	1A	3933	1/1	0.78	0.16	39,39,39,39	0
58	MG	1b	302	1/1	0.78	0.11	93,93,93,93	0
58	MG	2a	1782	1/1	0.78	0.13	97,97,97,97	0
58	MG	1A	3288	1/1	0.78	0.24	73,73,73,73	0
58	MG	1A	3214	1/1	0.78	0.20	59,59,59,59	0
58	MG	1A	3450	1/1	0.78	0.21	72,72,72,72	0
58	MG	2A	3156	1/1	0.78	0.19	74,74,74,74	0
58	MG	2a	1822	1/1	0.78	0.21	98,98,98,98	0
58	MG	2A	3059	1/1	0.78	0.25	80,80,80,80	0
58	MG	1A	3396	1/1	0.78	0.41	73,73,73,73	0
58	MG	28	103	1/1	0.78	0.13	84,84,84,84	0
58	MG	1A	3430	1/1	0.78	0.22	75,75,75,75	0
58	MG	2A	3595	1/1	0.79	0.28	58,58,58,58	0
58	MG	2A	3195	1/1	0.79	0.29	64,64,64,64	0
58	MG	1a	1802	1/1	0.79	0.09	78,78,78,78	0
58	MG	2a	1605	1/1	0.79	0.23	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3307	1/1	0.79	0.39	64,64,64,64	0
58	MG	2a	1609	1/1	0.79	0.13	80,80,80,80	0
58	MG	2A	3611	1/1	0.79	0.09	62,62,62,62	0
58	MG	2A	3203	1/1	0.79	0.19	68,68,68,68	0
58	MG	2A	3078	1/1	0.79	0.14	67,67,67,67	0
58	MG	1A	3632	1/1	0.79	0.12	64,64,64,64	0
58	MG	2A	3653	1/1	0.79	0.13	78,78,78,78	0
58	MG	1a	1666	1/1	0.79	0.11	86,86,86,86	0
58	MG	2A	3091	1/1	0.79	0.16	63,63,63,63	0
58	MG	1A	4059	1/1	0.79	0.25	57,57,57,57	0
58	MG	2A	3370	1/1	0.79	0.22	79,79,79,79	0
58	MG	1a	1674	1/1	0.79	0.21	69,69,69,69	0
58	MG	2a	1642	1/1	0.79	0.24	75,75,75,75	0
58	MG	2A	3236	1/1	0.79	0.19	89,89,89,89	0
58	MG	2A	3106	1/1	0.79	0.16	78,78,78,78	0
58	MG	1A	3502	1/1	0.79	0.24	70,70,70,70	0
58	MG	2A	3700	1/1	0.79	0.18	73,73,73,73	0
58	MG	1H	201	1/1	0.79	0.28	76,76,76,76	0
58	MG	1a	1682	1/1	0.79	0.21	64,64,64,64	0
58	MG	1A	3688	1/1	0.79	0.21	41,41,41,41	0
58	MG	1a	1687	1/1	0.79	0.21	76,76,76,76	0
58	MG	1x	102	1/1	0.79	0.22	67,67,67,67	0
58	MG	2A	3428	1/1	0.79	0.20	48,48,48,48	0
58	MG	1a	1691	1/1	0.79	0.20	78,78,78,78	0
58	MG	1a	1694	1/1	0.79	0.23	70,70,70,70	0
58	MG	1A	3916	1/1	0.79	0.12	54,54,54,54	0
58	MG	1A	3512	1/1	0.79	0.55	65,65,65,65	0
58	MG	2A	3282	1/1	0.79	0.16	75,75,75,75	0
58	MG	2A	3155	1/1	0.79	0.35	77,77,77,77	0
58	MG	1A	3044	1/1	0.79	0.15	50,50,50,50	0
58	MG	1A	4036	1/1	0.79	0.14	57,57,57,57	0
58	MG	2a	1764	1/1	0.79	0.18	97,97,97,97	0
58	MG	2a	1778	1/1	0.79	0.45	76,76,76,76	0
58	MG	1A	3737	1/1	0.79	0.19	44,44,44,44	0
58	MG	2A	3310	1/1	0.79	0.29	85,85,85,85	0
58	MG	2a	1785	1/1	0.79	0.14	80,80,80,80	0
58	MG	2A	3312	1/1	0.79	0.25	82,82,82,82	0
58	MG	1a	1623	1/1	0.79	0.14	84,84,84,84	0
58	MG	2A	3579	1/1	0.79	0.26	71,71,71,71	0
58	MG	2a	1805	1/1	0.79	0.12	88,88,88,88	0
58	MG	1B	220	1/1	0.79	0.17	65,65,65,65	0
58	MG	2A	3322	1/1	0.79	0.29	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2f	201	1/1	0.79	0.29	62,62,62,62	0
58	MG	2f	202	1/1	0.79	0.19	89,89,89,89	0
58	MG	1a	1631	1/1	0.79	0.12	80,80,80,80	0
58	MG	2q	201	1/1	0.79	0.22	81,81,81,81	0
58	MG	1A	3088	1/1	0.79	0.38	61,61,61,61	0
58	MG	1A	3983	1/1	0.79	0.14	61,61,61,61	0
58	MG	2x	103	1/1	0.79	0.32	86,86,86,86	0
58	MG	28	102	1/1	0.79	0.19	71,71,71,71	0
58	MG	2A	3212	1/1	0.80	0.16	65,65,65,65	0
58	MG	1A	3275	1/1	0.80	0.15	64,64,64,64	0
58	MG	2A	3223	1/1	0.80	0.48	75,75,75,75	0
58	MG	1F	307	1/1	0.80	0.23	60,60,60,60	0
58	MG	1A	3246	1/1	0.80	0.12	73,73,73,73	0
58	MG	1a	1639	1/1	0.80	0.07	79,79,79,79	0
58	MG	1a	1717	1/1	0.80	0.11	88,88,88,88	0
58	MG	1a	1644	1/1	0.80	0.07	79,79,79,79	0
58	MG	1a	1728	1/1	0.80	0.17	76,76,76,76	0
58	MG	1A	3342	1/1	0.80	0.17	68,68,68,68	0
58	MG	1A	3626	1/1	0.80	0.14	83,83,83,83	0
58	MG	1Q	206	1/1	0.80	0.18	69,69,69,69	0
58	MG	2A	3153	1/1	0.80	0.13	72,72,72,72	0
58	MG	2A	3389	1/1	0.80	0.72	71,71,71,71	0
58	MG	1A	3496	1/1	0.80	0.23	77,77,77,77	0
58	MG	2A	3052	1/1	0.80	0.09	65,65,65,65	0
58	MG	2a	1759	1/1	0.80	0.18	85,85,85,85	0
58	MG	10	105	1/1	0.80	0.28	69,69,69,69	0
58	MG	1A	3318	1/1	0.80	0.15	52,52,52,52	0
58	MG	1f	202	1/1	0.80	0.12	80,80,80,80	0
58	MG	1A	3506	1/1	0.80	0.13	66,66,66,66	0
58	MG	1a	1680	1/1	0.80	0.11	93,93,93,93	0
58	MG	1A	3372	1/1	0.80	0.19	55,55,55,55	0
58	MG	2A	3297	1/1	0.80	0.22	70,70,70,70	0
58	MG	2A	3303	1/1	0.80	0.14	86,86,86,86	0
58	MG	1A	3705	1/1	0.80	0.16	86,86,86,86	0
58	MG	2A	3489	1/1	0.80	0.14	85,85,85,85	0
58	MG	1a	1620	1/1	0.80	0.27	67,67,67,67	0
58	MG	1A	3382	1/1	0.80	0.30	55,55,55,55	0
58	MG	1A	3519	1/1	0.80	0.18	80,80,80,80	0
58	MG	2A	3099	1/1	0.80	0.24	77,77,77,77	0
58	MG	2A	3101	1/1	0.80	0.20	72,72,72,72	0
58	MG	1w	107	1/1	0.80	0.25	78,78,78,78	0
58	MG	1E	302	1/1	0.80	0.39	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	1641	1/1	0.80	0.11	81,81,81,81	0
58	MG	2A	3758	1/1	0.80	0.19	55,55,55,55	0
58	MG	2x	104	1/1	0.80	0.20	85,85,85,85	0
58	MG	2A	3574	1/1	0.80	0.10	53,53,53,53	0
58	MG	1a	1808	1/1	0.81	0.15	85,85,85,85	0
58	MG	1A	3819	1/1	0.81	0.14	58,58,58,58	0
58	MG	2A	3339	1/1	0.81	0.09	73,73,73,73	0
58	MG	1A	3962	1/1	0.81	0.10	79,79,79,79	0
58	MG	1N	202	1/1	0.81	0.24	53,53,53,53	0
58	MG	2A	3635	1/1	0.81	0.17	59,59,59,59	0
58	MG	1s	101	1/1	0.81	0.07	86,86,86,86	0
58	MG	2A	3226	1/1	0.81	0.51	68,68,68,68	0
58	MG	2A	3347	1/1	0.81	0.10	77,77,77,77	0
58	MG	2A	3228	1/1	0.81	0.39	74,74,74,74	0
58	MG	2A	3359	1/1	0.81	0.37	57,57,57,57	0
58	MG	1A	3397	1/1	0.81	0.14	72,72,72,72	0
58	MG	2A	3367	1/1	0.81	0.51	79,79,79,79	0
58	MG	2a	1644	1/1	0.81	0.20	76,76,76,76	0
58	MG	2a	1647	1/1	0.81	0.10	93,93,93,93	0
58	MG	2A	3230	1/1	0.81	0.64	84,84,84,84	0
58	MG	2a	1656	1/1	0.81	0.17	76,76,76,76	0
58	MG	1A	3836	1/1	0.81	0.16	78,78,78,78	0
58	MG	2A	3386	1/1	0.81	0.30	60,60,60,60	0
58	MG	1A	3316	1/1	0.81	0.35	82,82,82,82	0
58	MG	1a	1679	1/1	0.81	0.10	84,84,84,84	0
58	MG	2a	1688	1/1	0.81	0.16	75,75,75,75	0
58	MG	2A	3708	1/1	0.81	0.39	81,81,81,81	0
58	MG	12	102	1/1	0.81	0.26	56,56,56,56	0
58	MG	13	103	1/1	0.81	0.30	64,64,64,64	0
58	MG	2A	3731	1/1	0.81	0.47	69,69,69,69	0
58	MG	1A	3851	1/1	0.81	0.37	56,56,56,56	0
58	MG	1A	3459	1/1	0.81	0.43	58,58,58,58	0
58	MG	2A	3259	1/1	0.81	0.43	66,66,66,66	0
58	MG	1a	1602	1/1	0.81	0.11	79,79,79,79	0
58	MG	2A	3125	1/1	0.81	0.18	76,76,76,76	0
58	MG	1A	3992	1/1	0.81	0.14	62,62,62,62	0
58	MG	2a	1735	1/1	0.81	0.12	83,83,83,83	0
58	MG	1A	3484	1/1	0.81	0.24	65,65,65,65	0
58	MG	2a	1752	1/1	0.81	0.10	83,83,83,83	0
58	MG	2A	3780	1/1	0.81	0.18	80,80,80,80	0
58	MG	2A	3268	1/1	0.81	0.13	70,70,70,70	0
58	MG	1x	106	1/1	0.81	0.37	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1a	1617	1/1	0.81	0.08	74,74,74,74	0
58	MG	1a	1619	1/1	0.81	0.26	74,74,74,74	0
58	MG	2A	3519	1/1	0.81	0.24	50,50,50,50	0
58	MG	1A	3646	1/1	0.81	0.14	71,71,71,71	0
58	MG	1A	3061	1/1	0.81	0.28	58,58,58,58	0
58	MG	1A	3886	1/1	0.81	0.24	65,65,65,65	0
58	MG	2A	3293	1/1	0.81	0.20	77,77,77,77	0
58	MG	1B	229	1/1	0.81	0.14	93,93,93,93	0
58	MG	2A	3040	1/1	0.81	0.25	73,73,73,73	0
58	MG	1A	3195	1/1	0.81	0.38	77,77,77,77	0
58	MG	1A	3912	1/1	0.81	0.18	68,68,68,68	0
58	MG	1A	3186	1/1	0.81	0.48	54,54,54,54	0
58	MG	1A	3816	1/1	0.81	0.13	58,58,58,58	0
58	MG	2A	3058	1/1	0.81	0.24	80,80,80,80	0
58	MG	1A	3817	1/1	0.81	0.28	49,49,49,49	0
58	MG	1a	1777	1/1	0.81	0.15	82,82,82,82	0
58	MG	2A	3065	1/1	0.81	0.24	78,78,78,78	0
58	MG	1a	1791	1/1	0.81	0.21	65,65,65,65	0
58	MG	2A	3593	1/1	0.81	0.23	66,66,66,66	0
58	MG	1A	4048	1/1	0.81	0.16	47,47,47,47	0
58	MG	1A	3368	1/1	0.82	0.25	62,62,62,62	0
58	MG	1A	4005	1/1	0.82	0.19	44,44,44,44	0
58	MG	2a	1620	1/1	0.82	0.18	82,82,82,82	0
58	MG	2A	3227	1/1	0.82	0.52	62,62,62,62	0
58	MG	2a	1622	1/1	0.82	0.26	76,76,76,76	0
58	MG	2A	3651	1/1	0.82	0.15	80,80,80,80	0
58	MG	2A	3087	1/1	0.82	0.34	76,76,76,76	0
58	MG	2a	1629	1/1	0.82	0.19	65,65,65,65	0
58	MG	2A	3363	1/1	0.82	0.43	68,68,68,68	0
58	MG	1A	4011	1/1	0.82	0.24	68,68,68,68	0
58	MG	2A	3663	1/1	0.82	0.05	78,78,78,78	0
58	MG	2A	3093	1/1	0.82	0.24	82,82,82,82	0
58	MG	2A	3097	1/1	0.82	0.17	75,75,75,75	0
58	MG	1n	101	1/1	0.82	0.13	77,77,77,77	0
58	MG	1A	3164	1/1	0.82	0.34	71,71,71,71	0
58	MG	1a	1673	1/1	0.82	0.20	75,75,75,75	0
58	MG	1A	3225	1/1	0.82	0.18	43,43,43,43	0
58	MG	2A	3254	1/1	0.82	0.23	82,82,82,82	0
58	MG	2A	3698	1/1	0.82	0.20	66,66,66,66	0
58	MG	1A	3415	1/1	0.82	0.43	56,56,56,56	0
58	MG	2A	3701	1/1	0.82	0.11	82,82,82,82	0
58	MG	1A	3323	1/1	0.82	0.26	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2a	1672	1/1	0.82	0.14	77,77,77,77	0
58	MG	1A	3532	1/1	0.82	0.29	46,46,46,46	0
58	MG	2a	1679	1/1	0.82	0.19	78,78,78,78	0
58	MG	2a	1685	1/1	0.82	0.11	84,84,84,84	0
58	MG	1N	205	1/1	0.82	0.27	60,60,60,60	0
58	MG	2A	3115	1/1	0.82	0.11	79,79,79,79	0
58	MG	2A	3118	1/1	0.82	0.18	89,89,89,89	0
58	MG	2A	3427	1/1	0.82	0.13	71,71,71,71	0
58	MG	1A	4038	1/1	0.82	0.14	48,48,48,48	0
58	MG	1A	3325	1/1	0.82	0.23	61,61,61,61	0
58	MG	1A	3751	1/1	0.82	0.21	38,38,38,38	0
58	MG	2a	1710	1/1	0.82	0.15	78,78,78,78	0
58	MG	1A	3079	1/1	0.82	0.30	62,62,62,62	0
58	MG	1A	3392	1/1	0.82	0.20	65,65,65,65	0
58	MG	1a	1702	1/1	0.82	0.44	71,71,71,71	0
58	MG	2A	3003	1/1	0.82	0.33	65,65,65,65	0
58	MG	1A	4054	1/1	0.82	0.13	64,64,64,64	0
58	MG	2A	3291	1/1	0.82	0.34	82,82,82,82	0
58	MG	2A	3796	1/1	0.82	0.29	59,59,59,59	0
58	MG	1A	4057	1/1	0.82	0.19	80,80,80,80	0
58	MG	2B	204	1/1	0.82	0.18	83,83,83,83	0
58	MG	1A	3930	1/1	0.82	0.08	66,66,66,66	0
58	MG	2B	206	1/1	0.82	0.35	73,73,73,73	0
58	MG	1A	3495	1/1	0.82	0.12	78,78,78,78	0
58	MG	1A	3944	1/1	0.82	0.07	68,68,68,68	0
58	MG	1a	1715	1/1	0.82	0.22	69,69,69,69	0
58	MG	2D	305	1/1	0.82	0.54	70,70,70,70	0
58	MG	1A	3328	1/1	0.82	0.27	70,70,70,70	0
58	MG	2a	1797	1/1	0.82	0.12	76,76,76,76	0
58	MG	1a	1726	1/1	0.82	0.21	52,52,52,52	0
58	MG	1A	3953	1/1	0.82	0.29	61,61,61,61	0
58	MG	1A	3157	1/1	0.82	0.20	38,38,38,38	0
58	MG	2a	1815	1/1	0.82	0.15	85,85,85,85	0
58	MG	2A	3054	1/1	0.82	0.30	76,76,76,76	0
58	MG	1A	3363	1/1	0.82	0.27	55,55,55,55	0
58	MG	1A	3451	1/1	0.82	0.24	55,55,55,55	0
58	MG	1A	3615	1/1	0.82	0.24	31,31,31,31	0
58	MG	1A	3821	1/1	0.82	0.27	68,68,68,68	0
58	MG	2I	202	1/1	0.82	0.19	88,88,88,88	0
58	MG	2A	3064	1/1	0.82	0.17	87,87,87,87	0
58	MG	1B	224	1/1	0.82	0.18	74,74,74,74	0
58	MG	2A	3602	1/1	0.82	0.21	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	2x	101	1/1	0.82	0.19	79,79,79,79	0
58	MG	1A	3340	1/1	0.82	0.26	63,63,63,63	0
58	MG	1A	3629	1/1	0.82	0.16	46,46,46,46	0
58	MG	1A	3518	1/1	0.82	0.31	82,82,82,82	0
58	MG	1A	3564	1/1	0.83	0.20	58,58,58,58	0
58	MG	2A	3777	1/1	0.83	0.27	91,91,91,91	0
58	MG	1A	3733	1/1	0.83	0.22	55,55,55,55	0
58	MG	1A	3093	1/1	0.83	0.32	60,60,60,60	0
58	MG	2a	1665	1/1	0.83	0.17	61,61,61,61	0
58	MG	2A	3124	1/1	0.83	0.25	73,73,73,73	0
58	MG	2a	1671	1/1	0.83	0.37	78,78,78,78	0
58	MG	1A	3200	1/1	0.83	0.17	43,43,43,43	0
58	MG	2A	3128	1/1	0.83	0.14	75,75,75,75	0
58	MG	1T	202	1/1	0.83	0.30	67,67,67,67	0
58	MG	1W	203	1/1	0.83	0.22	55,55,55,55	0
58	MG	1A	3270	1/1	0.83	0.23	51,51,51,51	0
58	MG	2A	3351	1/1	0.83	0.29	77,77,77,77	0
58	MG	2a	1699	1/1	0.83	0.13	74,74,74,74	0
58	MG	1A	4073	1/1	0.83	0.21	63,63,63,63	0
58	MG	1A	3528	1/1	0.83	0.12	69,69,69,69	0
58	MG	2A	3260	1/1	0.83	0.44	69,69,69,69	0
58	MG	1A	3762	1/1	0.83	0.18	41,41,41,41	0
58	MG	1A	3773	1/1	0.83	0.13	95,95,95,95	0
58	MG	2E	308	1/1	0.83	0.27	55,55,55,55	0
58	MG	2F	303	1/1	0.83	0.22	83,83,83,83	0
58	MG	2F	304	1/1	0.83	0.21	78,78,78,78	0
58	MG	1A	3029	1/1	0.83	0.24	46,46,46,46	0
58	MG	1B	212	1/1	0.83	0.14	73,73,73,73	0
58	MG	1A	3120	1/1	0.83	0.72	56,56,56,56	0
58	MG	2A	3387	1/1	0.83	0.65	77,77,77,77	0
58	MG	1a	1692	1/1	0.83	0.29	74,74,74,74	0
58	MG	1A	3924	1/1	0.83	0.21	41,41,41,41	0
58	MG	25	101	1/1	0.83	0.28	65,65,65,65	0
58	MG	2A	3391	1/1	0.83	0.28	69,69,69,69	0
58	MG	1A	3026	1/1	0.83	0.20	64,64,64,64	0
58	MG	2A	3655	1/1	0.83	0.20	81,81,81,81	0
58	MG	1A	3217	1/1	0.83	0.24	84,84,84,84	0
58	MG	1a	1709	1/1	0.83	0.24	72,72,72,72	0
58	MG	2A	3286	1/1	0.83	0.29	83,83,83,83	0
58	MG	1A	3934	1/1	0.83	0.06	71,71,71,71	0
58	MG	2A	3289	1/1	0.83	0.21	75,75,75,75	0
58	MG	1A	3361	1/1	0.83	0.29	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3333	1/1	0.83	0.36	71,71,71,71	0
58	MG	1A	4045	1/1	0.83	0.09	76,76,76,76	0
58	MG	1A	3671	1/1	0.83	0.23	40,40,40,40	0
58	MG	2A	3306	1/1	0.83	0.24	69,69,69,69	0
58	MG	1A	3557	1/1	0.83	0.35	73,73,73,73	0
58	MG	2A	3707	1/1	0.83	0.07	73,73,73,73	0
58	MG	2A	3485	1/1	0.83	0.25	43,43,43,43	0
58	MG	2A	3002	1/1	0.83	0.50	70,70,70,70	0
58	MG	1a	1721	1/1	0.83	0.22	72,72,72,72	0
58	MG	2A	3214	1/1	0.83	0.38	52,52,52,52	0
58	MG	2A	3109	1/1	0.83	0.19	71,71,71,71	0
58	MG	1A	3558	1/1	0.83	0.28	65,65,65,65	0
58	MG	2A	3324	1/1	0.83	0.21	77,77,77,77	0
58	MG	1a	1641	1/1	0.83	0.14	69,69,69,69	0
58	MG	1A	3224	1/1	0.83	0.17	55,55,55,55	0
58	MG	1a	1735	1/1	0.83	0.14	71,71,71,71	0
58	MG	1a	1655	1/1	0.84	0.07	69,69,69,69	0
58	MG	1a	1661	1/1	0.84	0.09	88,88,88,88	0
58	MG	1A	3260	1/1	0.84	0.12	66,66,66,66	0
58	MG	2A	3272	1/1	0.84	0.43	82,82,82,82	0
58	MG	1R	203	1/1	0.84	0.19	64,64,64,64	0
58	MG	1a	1772	1/1	0.84	0.23	74,74,74,74	0
58	MG	2A	3401	1/1	0.84	0.61	66,66,66,66	0
58	MG	1A	3289	1/1	0.84	0.39	67,67,67,67	0
58	MG	2A	3406	1/1	0.84	0.58	76,76,76,76	0
58	MG	1a	1779	1/1	0.84	0.11	71,71,71,71	0
58	MG	1A	3622	1/1	0.84	0.29	68,68,68,68	0
58	MG	2A	3170	1/1	0.84	0.19	53,53,53,53	0
58	MG	2a	1653	1/1	0.84	0.10	73,73,73,73	0
58	MG	1a	1799	1/1	0.84	0.10	89,89,89,89	0
58	MG	1A	3319	1/1	0.84	0.25	68,68,68,68	0
58	MG	2A	3733	1/1	0.84	0.17	72,72,72,72	0
58	MG	2a	1660	1/1	0.84	0.09	86,86,86,86	0
58	MG	2A	3438	1/1	0.84	0.10	61,61,61,61	0
58	MG	1A	3420	1/1	0.84	0.11	76,76,76,76	0
58	MG	1A	4000	1/1	0.84	0.06	94,94,94,94	0
58	MG	1A	3893	1/1	0.84	0.21	67,67,67,67	0
58	MG	2A	3076	1/1	0.84	0.40	62,62,62,62	0
58	MG	1A	3250	1/1	0.84	0.24	55,55,55,55	0
58	MG	1A	3784	1/1	0.84	0.12	60,60,60,60	0
58	MG	2A	3770	1/1	0.84	0.20	61,61,61,61	0
58	MG	1a	1601	1/1	0.84	0.28	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3084	1/1	0.84	0.27	67,67,67,67	0
58	MG	2A	3315	1/1	0.84	0.24	80,80,80,80	0
58	MG	1A	3429	1/1	0.84	0.22	77,77,77,77	0
58	MG	1A	3798	1/1	0.84	0.24	41,41,41,41	0
58	MG	2A	3559	1/1	0.84	0.51	82,82,82,82	0
58	MG	2A	3798	1/1	0.84	0.11	74,74,74,74	0
58	MG	1A	3165	1/1	0.84	0.22	40,40,40,40	0
58	MG	2A	3095	1/1	0.84	0.17	63,63,63,63	0
58	MG	2A	3566	1/1	0.84	0.14	82,82,82,82	0
58	MG	2A	3568	1/1	0.84	0.21	61,61,61,61	0
58	MG	2A	3217	1/1	0.84	0.18	71,71,71,71	0
58	MG	1A	3300	1/1	0.84	0.36	44,44,44,44	0
58	MG	2a	1736	1/1	0.84	0.20	83,83,83,83	0
58	MG	1a	1695	1/1	0.84	0.27	63,63,63,63	0
58	MG	2A	3224	1/1	0.84	0.24	66,66,66,66	0
58	MG	2a	1753	1/1	0.84	0.10	88,88,88,88	0
58	MG	2E	302	1/1	0.84	0.09	71,71,71,71	0
58	MG	1a	1618	1/1	0.84	0.13	58,58,58,58	0
58	MG	1A	3679	1/1	0.84	0.15	35,35,35,35	0
58	MG	1a	1708	1/1	0.84	0.10	98,98,98,98	0
58	MG	1A	3257	1/1	0.84	0.18	44,44,44,44	0
58	MG	1A	3939	1/1	0.84	0.20	91,91,91,91	0
58	MG	1A	4040	1/1	0.84	0.12	55,55,55,55	0
58	MG	2a	1784	1/1	0.84	0.23	81,81,81,81	0
58	MG	1a	1628	1/1	0.84	0.30	68,68,68,68	0
58	MG	1x	107	1/1	0.84	0.28	71,71,71,71	0
58	MG	1x	112	1/1	0.84	0.08	67,67,67,67	0
58	MG	2A	3605	1/1	0.84	0.18	71,71,71,71	0
58	MG	2A	3249	1/1	0.84	0.19	84,84,84,84	0
58	MG	1A	3481	1/1	0.84	0.28	58,58,58,58	0
58	MG	2a	1806	1/1	0.84	0.34	87,87,87,87	0
58	MG	2A	3362	1/1	0.84	0.40	49,49,49,49	0
58	MG	1E	312	1/1	0.84	0.14	66,66,66,66	0
58	MG	1A	3828	1/1	0.84	0.30	69,69,69,69	0
58	MG	2d	302	1/1	0.84	0.07	67,67,67,67	0
58	MG	2A	3638	1/1	0.84	0.22	70,70,70,70	0
58	MG	1A	3574	1/1	0.84	0.29	63,63,63,63	0
58	MG	2A	3650	1/1	0.84	0.28	64,64,64,64	0
58	MG	2A	3368	1/1	0.84	0.27	71,71,71,71	0
58	MG	1A	3580	1/1	0.84	0.17	50,50,50,50	0
58	MG	2a	1614	1/1	0.84	0.37	73,73,73,73	0
58	MG	1A	3963	1/1	0.84	0.36	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3374	1/1	0.84	0.36	71,71,71,71	0
58	MG	2A	3376	1/1	0.84	0.48	69,69,69,69	0
58	MG	1A	3408	1/1	0.84	0.44	59,59,59,59	0
58	MG	1A	3180	1/1	0.84	0.31	58,58,58,58	0
58	MG	2x	107	1/1	0.84	0.25	80,80,80,80	0
58	MG	2A	3283	1/1	0.85	0.56	63,63,63,63	0
58	MG	1A	3549	1/1	0.85	0.27	64,64,64,64	0
58	MG	1A	4013	1/1	0.85	0.09	51,51,51,51	0
58	MG	1A	4017	1/1	0.85	0.37	89,89,89,89	0
58	MG	2A	3171	1/1	0.85	0.19	70,70,70,70	0
58	MG	1A	3696	1/1	0.85	0.28	59,59,59,59	0
58	MG	1A	3314	1/1	0.85	0.27	61,61,61,61	0
58	MG	1A	3443	1/1	0.85	0.50	50,50,50,50	0
58	MG	1A	3446	1/1	0.85	0.41	47,47,47,47	0
58	MG	2A	3455	1/1	0.85	0.13	67,67,67,67	0
58	MG	2A	3730	1/1	0.85	0.15	74,74,74,74	0
58	MG	1A	3447	1/1	0.85	0.27	60,60,60,60	0
58	MG	1a	1805	1/1	0.85	0.20	79,79,79,79	0
58	MG	1Q	201	1/1	0.85	0.58	49,49,49,49	0
58	MG	1A	3055	1/1	0.85	0.25	56,56,56,56	0
58	MG	2A	3745	1/1	0.85	0.15	71,71,71,71	0
58	MG	1A	3754	1/1	0.85	0.15	65,65,65,65	0
58	MG	2A	3513	1/1	0.85	0.22	84,84,84,84	0
58	MG	2A	3516	1/1	0.85	0.15	66,66,66,66	0
58	MG	2A	3517	1/1	0.85	0.34	74,74,74,74	0
58	MG	1A	3206	1/1	0.85	0.21	44,44,44,44	0
58	MG	1A	3290	1/1	0.85	0.19	61,61,61,61	0
58	MG	2a	1681	1/1	0.85	0.10	80,80,80,80	0
58	MG	1A	3346	1/1	0.85	0.38	60,60,60,60	0
58	MG	1A	3516	1/1	0.85	0.22	73,73,73,73	0
58	MG	2A	3323	1/1	0.85	0.13	79,79,79,79	0
58	MG	2a	1697	1/1	0.85	0.18	86,86,86,86	0
58	MG	1A	3775	1/1	0.85	0.17	64,64,64,64	0
58	MG	2A	3216	1/1	0.85	0.21	74,74,74,74	0
58	MG	1a	1688	1/1	0.85	0.32	74,74,74,74	0
58	MG	2A	3218	1/1	0.85	0.21	57,57,57,57	0
58	MG	2A	3800	1/1	0.85	0.15	86,86,86,86	0
58	MG	1A	3453	1/1	0.85	0.24	58,58,58,58	0
58	MG	2A	3570	1/1	0.85	0.35	79,79,79,79	0
58	MG	1A	3608	1/1	0.85	0.17	64,64,64,64	0
58	MG	1a	1693	1/1	0.85	0.14	80,80,80,80	0
58	MG	2a	1717	1/1	0.85	0.22	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2B	207	1/1	0.85	0.26	77,77,77,77	0
58	MG	2B	209	1/1	0.85	0.13	81,81,81,81	0
58	MG	1A	3411	1/1	0.85	0.12	68,68,68,68	0
58	MG	1A	3797	1/1	0.85	0.20	77,77,77,77	0
58	MG	1A	3163	1/1	0.85	0.25	67,67,67,67	0
58	MG	1A	3949	1/1	0.85	0.22	54,54,54,54	0
58	MG	1A	3799	1/1	0.85	0.12	64,64,64,64	0
58	MG	1A	3101	1/1	0.85	0.18	85,85,85,85	0
58	MG	2a	1756	1/1	0.85	0.13	85,85,85,85	0
58	MG	2A	3234	1/1	0.85	0.31	73,73,73,73	0
58	MG	1A	3815	1/1	0.85	0.25	64,64,64,64	0
58	MG	1A	3467	1/1	0.85	0.19	79,79,79,79	0
58	MG	2F	305	1/1	0.85	0.21	66,66,66,66	0
58	MG	1A	3968	1/1	0.85	0.14	85,85,85,85	0
58	MG	1A	3255	1/1	0.85	0.13	73,73,73,73	0
58	MG	1A	3472	1/1	0.85	0.15	78,78,78,78	0
58	MG	1A	3151	1/1	0.85	0.27	45,45,45,45	0
58	MG	1A	3826	1/1	0.85	0.17	73,73,73,73	0
58	MG	1A	3357	1/1	0.85	0.14	69,69,69,69	0
58	MG	2A	3023	1/1	0.85	0.11	84,84,84,84	0
58	MG	25	102	1/1	0.85	0.29	63,63,63,63	0
58	MG	2A	3626	1/1	0.85	0.14	42,42,42,42	0
58	MG	28	101	1/1	0.85	0.10	65,65,65,65	0
58	MG	2a	1810	1/1	0.85	0.23	76,76,76,76	0
58	MG	2A	3130	1/1	0.85	0.22	65,65,65,65	0
58	MG	2a	1818	1/1	0.85	0.12	83,83,83,83	0
58	MG	1A	3313	1/1	0.85	0.26	74,74,74,74	0
58	MG	2A	3377	1/1	0.85	0.56	77,77,77,77	0
58	MG	2A	3383	1/1	0.85	0.28	66,66,66,66	0
58	MG	2A	3384	1/1	0.85	0.22	58,58,58,58	0
58	MG	2A	3033	1/1	0.85	0.19	53,53,53,53	0
58	MG	1A	3330	1/1	0.85	0.22	61,61,61,61	0
58	MG	2a	1610	1/1	0.85	0.14	72,72,72,72	0
58	MG	2A	3037	1/1	0.85	0.28	74,74,74,74	0
58	MG	1A	3690	1/1	0.85	0.14	47,47,47,47	0
58	MG	2A	3662	1/1	0.85	0.12	64,64,64,64	0
58	MG	1A	3846	1/1	0.85	0.26	71,71,71,71	0
58	MG	2A	3275	1/1	0.85	0.23	74,74,74,74	0
58	MG	2A	3047	1/1	0.85	0.12	68,68,68,68	0
58	MG	1a	1642	1/1	0.85	0.25	82,82,82,82	0
58	MG	2A	3161	1/1	0.85	0.12	64,64,64,64	0
58	MG	1A	3364	1/1	0.86	0.35	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2a	1628	1/1	0.86	0.11	93,93,93,93	0
58	MG	1x	108	1/1	0.86	0.14	90,90,90,90	0
58	MG	1A	3537	1/1	0.86	0.18	37,37,37,37	0
58	MG	2A	3684	1/1	0.86	0.09	73,73,73,73	0
58	MG	1A	3452	1/1	0.86	0.20	78,78,78,78	0
58	MG	2a	1635	1/1	0.86	0.23	76,76,76,76	0
58	MG	1A	3266	1/1	0.86	0.43	63,63,63,63	0
58	MG	2A	3398	1/1	0.86	0.34	52,52,52,52	0
58	MG	1A	4004	1/1	0.86	0.12	37,37,37,37	0
58	MG	2A	3265	1/1	0.86	0.26	84,84,84,84	0
58	MG	1A	3087	1/1	0.86	0.30	47,47,47,47	0
58	MG	1A	3900	1/1	0.86	0.21	31,31,31,31	0
58	MG	2a	1648	1/1	0.86	0.29	81,81,81,81	0
58	MG	1A	3649	1/1	0.86	0.25	39,39,39,39	0
58	MG	2A	3408	1/1	0.86	0.24	83,83,83,83	0
58	MG	2A	3138	1/1	0.86	0.21	48,48,48,48	0
58	MG	2A	3721	1/1	0.86	0.09	72,72,72,72	0
58	MG	1A	3650	1/1	0.86	0.20	33,33,33,33	0
58	MG	2A	3142	1/1	0.86	0.40	68,68,68,68	0
58	MG	2A	3144	1/1	0.86	0.25	53,53,53,53	0
58	MG	1a	1629	1/1	0.86	0.11	71,71,71,71	0
58	MG	1A	3064	1/1	0.86	0.21	66,66,66,66	0
58	MG	1A	3402	1/1	0.86	0.25	72,72,72,72	0
58	MG	1A	3435	1/1	0.86	0.19	61,61,61,61	0
58	MG	1a	1729	1/1	0.86	0.18	66,66,66,66	0
58	MG	1D	3606	1/1	0.86	0.23	45,45,45,45	0
58	MG	1A	4033	1/1	0.86	0.26	79,79,79,79	0
58	MG	1A	4035	1/1	0.86	0.08	53,53,53,53	0
58	MG	2A	3499	1/1	0.86	0.21	82,82,82,82	0
58	MG	2a	1696	1/1	0.86	0.08	85,85,85,85	0
58	MG	1a	1750	1/1	0.86	0.18	65,65,65,65	0
58	MG	1A	3562	1/1	0.86	0.25	37,37,37,37	0
58	MG	2A	3188	1/1	0.86	0.22	69,69,69,69	0
58	MG	2a	1703	1/1	0.86	0.13	74,74,74,74	0
58	MG	1A	3345	1/1	0.86	0.22	69,69,69,69	0
58	MG	2A	3530	1/1	0.86	0.19	75,75,75,75	0
58	MG	1F	309	1/1	0.86	0.21	48,48,48,48	0
58	MG	1a	1775	1/1	0.86	0.20	78,78,78,78	0
58	MG	1a	1648	1/1	0.86	0.15	71,71,71,71	0
58	MG	1a	1649	1/1	0.86	0.12	73,73,73,73	0
58	MG	1a	1782	1/1	0.86	0.10	85,85,85,85	0
58	MG	2A	3561	1/1	0.86	0.22	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3318	1/1	0.86	0.14	63,63,63,63	0
58	MG	1A	3256	1/1	0.86	0.25	37,37,37,37	0
58	MG	1A	3374	1/1	0.86	0.36	63,63,63,63	0
58	MG	1a	1662	1/1	0.86	0.14	78,78,78,78	0
58	MG	1A	3703	1/1	0.86	0.25	44,44,44,44	0
58	MG	1A	3377	1/1	0.86	0.19	68,68,68,68	0
58	MG	2A	3211	1/1	0.86	0.16	69,69,69,69	0
58	MG	1A	4042	1/1	0.86	0.24	42,42,42,42	0
58	MG	1f	201	1/1	0.86	0.22	61,61,61,61	0
58	MG	2A	3215	1/1	0.86	0.26	68,68,68,68	0
58	MG	2a	1760	1/1	0.86	0.09	90,90,90,90	0
58	MG	2A	3086	1/1	0.86	0.22	71,71,71,71	0
58	MG	1A	3707	1/1	0.86	0.27	66,66,66,66	0
58	MG	2A	3088	1/1	0.86	0.26	74,74,74,74	0
58	MG	1A	3479	1/1	0.86	0.21	61,61,61,61	0
58	MG	1Q	208	1/1	0.86	0.43	59,59,59,59	0
58	MG	2A	3345	1/1	0.86	0.17	86,86,86,86	0
58	MG	1A	3381	1/1	0.86	0.22	63,63,63,63	0
58	MG	1A	4052	1/1	0.86	0.18	83,83,83,83	0
58	MG	1A	3832	1/1	0.86	0.24	72,72,72,72	0
58	MG	2a	1799	1/1	0.86	0.18	83,83,83,83	0
58	MG	20	102	1/1	0.86	0.19	72,72,72,72	0
58	MG	1U	203	1/1	0.86	0.55	64,64,64,64	0
58	MG	1V	203	1/1	0.86	0.36	45,45,45,45	0
58	MG	1A	3305	1/1	0.86	0.24	56,56,56,56	0
58	MG	2A	3619	1/1	0.86	0.26	67,67,67,67	0
58	MG	2a	1812	1/1	0.86	0.33	87,87,87,87	0
58	MG	2a	1814	1/1	0.86	0.23	75,75,75,75	0
58	MG	1A	3187	1/1	0.86	0.27	58,58,58,58	0
58	MG	2A	3364	1/1	0.86	0.19	59,59,59,59	0
58	MG	2A	3233	1/1	0.86	0.28	84,84,84,84	0
58	MG	1A	3753	1/1	0.86	0.19	27,27,27,27	0
58	MG	2d	301	1/1	0.86	0.37	69,69,69,69	0
58	MG	2a	1604	1/1	0.86	0.23	72,72,72,72	0
58	MG	2A	3235	1/1	0.86	0.35	77,77,77,77	0
58	MG	1A	3611	1/1	0.86	0.09	38,38,38,38	0
58	MG	1A	4064	1/1	0.86	0.16	50,50,50,50	0
58	MG	2A	3241	1/1	0.86	0.27	77,77,77,77	0
58	MG	1A	3859	1/1	0.86	0.51	56,56,56,56	0
58	MG	2A	3244	1/1	0.86	0.22	79,79,79,79	0
58	MG	2a	1617	1/1	0.86	0.14	82,82,82,82	0
58	MG	1A	3486	1/1	0.86	0.19	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3250	1/1	0.86	0.21	69,69,69,69	0
58	MG	1A	4070	1/1	0.86	0.17	72,72,72,72	0
58	MG	2A	3669	1/1	0.86	0.26	63,63,63,63	0
58	MG	2A	3119	1/1	0.86	0.39	76,76,76,76	0
58	MG	2x	108	1/1	0.86	0.23	79,79,79,79	0
59	K	2A	3403	1/1	0.86	0.15	84,84,84,84	0
58	MG	1A	4047	1/1	0.87	0.12	59,59,59,59	0
58	MG	17	105	1/1	0.87	0.22	64,64,64,64	0
58	MG	1A	3309	1/1	0.87	0.27	59,59,59,59	0
58	MG	2A	3208	1/1	0.87	0.43	80,80,80,80	0
58	MG	2A	3349	1/1	0.87	0.22	66,66,66,66	0
58	MG	1A	3312	1/1	0.87	0.21	69,69,69,69	0
58	MG	1A	3048	1/1	0.87	0.22	54,54,54,54	0
58	MG	1A	3230	1/1	0.87	0.24	59,59,59,59	0
58	MG	1a	1603	1/1	0.87	0.10	67,67,67,67	0
58	MG	1A	3785	1/1	0.87	0.28	59,59,59,59	0
58	MG	1A	3936	1/1	0.87	0.13	61,61,61,61	0
58	MG	1a	1615	1/1	0.87	0.12	81,81,81,81	0
58	MG	1A	3062	1/1	0.87	0.27	61,61,61,61	0
58	MG	2A	3220	1/1	0.87	0.19	59,59,59,59	0
58	MG	1A	3456	1/1	0.87	0.28	69,69,69,69	0
58	MG	1A	3267	1/1	0.87	0.28	69,69,69,69	0
58	MG	1A	3152	1/1	0.87	0.32	56,56,56,56	0
58	MG	1A	3155	1/1	0.87	0.32	51,51,51,51	0
58	MG	1A	3956	1/1	0.87	0.14	70,70,70,70	0
58	MG	2A	3686	1/1	0.87	0.17	71,71,71,71	0
58	MG	2a	1654	1/1	0.87	0.22	81,81,81,81	0
58	MG	2A	3379	1/1	0.87	0.33	70,70,70,70	0
58	MG	2A	3382	1/1	0.87	0.16	87,87,87,87	0
58	MG	1A	3019	1/1	0.87	0.28	57,57,57,57	0
58	MG	1A	3468	1/1	0.87	0.30	74,74,74,74	0
58	MG	1a	1781	1/1	0.87	0.21	85,85,85,85	0
58	MG	1A	4078	1/1	0.87	0.12	54,54,54,54	0
58	MG	2a	1668	1/1	0.87	0.21	67,67,67,67	0
58	MG	1A	3158	1/1	0.87	0.32	66,66,66,66	0
58	MG	1a	1792	1/1	0.87	0.16	58,58,58,58	0
58	MG	1A	3005	1/1	0.87	0.15	55,55,55,55	0
58	MG	1A	3973	1/1	0.87	0.15	89,89,89,89	0
58	MG	1A	3820	1/1	0.87	0.16	79,79,79,79	0
58	MG	1B	214	1/1	0.87	0.17	54,54,54,54	0
58	MG	2A	3243	1/1	0.87	0.31	83,83,83,83	0
58	MG	1A	3684	1/1	0.87	0.18	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	1d	301	1/1	0.87	0.51	74,74,74,74	0
58	MG	1A	3366	1/1	0.87	0.15	55,55,55,55	0
58	MG	1A	3212	1/1	0.87	0.15	44,44,44,44	0
58	MG	2a	1701	1/1	0.87	0.23	81,81,81,81	0
58	MG	1A	3829	1/1	0.87	0.20	60,60,60,60	0
58	MG	1A	3995	1/1	0.87	0.36	45,45,45,45	0
58	MG	2A	3414	1/1	0.87	0.21	62,62,62,62	0
58	MG	2A	3418	1/1	0.87	0.21	78,78,78,78	0
58	MG	2A	3767	1/1	0.87	0.05	85,85,85,85	0
58	MG	1A	3422	1/1	0.87	0.39	68,68,68,68	0
58	MG	1a	1656	1/1	0.87	0.22	76,76,76,76	0
58	MG	1A	3295	1/1	0.87	0.15	77,77,77,77	0
58	MG	1A	3331	1/1	0.87	0.19	51,51,51,51	0
58	MG	2a	1716	1/1	0.87	0.26	76,76,76,76	0
58	MG	2A	3447	1/1	0.87	0.15	48,48,48,48	0
58	MG	2A	3786	1/1	0.87	0.23	56,56,56,56	0
58	MG	1A	3296	1/1	0.87	0.18	67,67,67,67	0
58	MG	1A	3297	1/1	0.87	0.18	44,44,44,44	0
58	MG	1A	3708	1/1	0.87	0.17	77,77,77,77	0
58	MG	2A	3466	1/1	0.87	0.23	51,51,51,51	0
58	MG	1A	3711	1/1	0.87	0.14	51,51,51,51	0
58	MG	1A	3861	1/1	0.87	0.42	43,43,43,43	0
58	MG	1A	3138	1/1	0.87	0.21	63,63,63,63	0
58	MG	2A	3273	1/1	0.87	0.61	81,81,81,81	0
58	MG	1A	3098	1/1	0.87	0.31	51,51,51,51	0
58	MG	1A	3877	1/1	0.87	0.13	38,38,38,38	0
58	MG	1A	4029	1/1	0.87	0.13	69,69,69,69	0
58	MG	1A	3578	1/1	0.87	0.26	48,48,48,48	0
58	MG	1A	3172	1/1	0.87	0.23	52,52,52,52	0
58	MG	2A	3528	1/1	0.87	0.22	65,65,65,65	0
58	MG	1A	3385	1/1	0.87	0.17	52,52,52,52	0
58	MG	1A	3583	1/1	0.87	0.29	60,60,60,60	0
58	MG	1R	207	1/1	0.87	0.25	50,50,50,50	0
58	MG	2a	1792	1/1	0.87	0.28	72,72,72,72	0
58	MG	1A	3386	1/1	0.87	0.20	53,53,53,53	0
58	MG	2A	3157	1/1	0.87	0.28	62,62,62,62	0
58	MG	2A	3158	1/1	0.87	0.22	83,83,83,83	0
58	MG	2A	3006	1/1	0.87	0.15	73,73,73,73	0
58	MG	2A	3162	1/1	0.87	0.09	74,74,74,74	0
58	MG	2A	3164	1/1	0.87	0.30	88,88,88,88	0
58	MG	1A	3060	1/1	0.87	0.16	73,73,73,73	0
58	MG	2A	3017	1/1	0.87	0.48	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	2W	201	1/1	0.87	0.19	79,79,79,79	0
58	MG	1A	3911	1/1	0.87	0.07	51,51,51,51	0
58	MG	2A	3572	1/1	0.87	0.26	82,82,82,82	0
58	MG	1U	206	1/1	0.87	0.34	42,42,42,42	0
58	MG	2A	3178	1/1	0.87	0.17	76,76,76,76	0
58	MG	2A	3182	1/1	0.87	0.58	78,78,78,78	0
58	MG	25	104	1/1	0.87	0.21	63,63,63,63	0
58	MG	2A	3183	1/1	0.87	0.48	77,77,77,77	0
58	MG	1a	1699	1/1	0.87	0.28	60,60,60,60	0
58	MG	2A	3320	1/1	0.87	0.26	79,79,79,79	0
58	MG	2A	3185	1/1	0.87	0.58	75,75,75,75	0
58	MG	1U	210	1/1	0.87	0.32	64,64,64,64	0
58	MG	2A	3032	1/1	0.87	0.25	69,69,69,69	0
58	MG	1a	1704	1/1	0.87	0.21	72,72,72,72	0
58	MG	2A	3192	1/1	0.87	0.21	65,65,65,65	0
58	MG	1A	3592	1/1	0.87	0.13	37,37,37,37	0
58	MG	1V	206	1/1	0.87	0.21	55,55,55,55	0
58	MG	1A	3766	1/1	0.87	0.05	78,78,78,78	0
58	MG	1A	4044	1/1	0.87	0.23	33,33,33,33	0
58	MG	1l	103	1/1	0.87	0.14	48,48,48,48	0
58	MG	2A	3202	1/1	0.87	0.17	76,76,76,76	0
58	MG	1A	3915	1/1	0.87	0.20	40,40,40,40	0
58	MG	2A	3771	1/1	0.88	0.12	53,53,53,53	0
58	MG	1A	3103	1/1	0.88	0.38	49,49,49,49	0
58	MG	2A	3779	1/1	0.88	0.30	86,86,86,86	0
58	MG	1A	3251	1/1	0.88	0.17	71,71,71,71	0
58	MG	1A	3867	1/1	0.88	0.18	34,34,34,34	0
58	MG	1B	231	1/1	0.88	0.13	82,82,82,82	0
58	MG	2A	3245	1/1	0.88	0.44	75,75,75,75	0
58	MG	1A	3871	1/1	0.88	0.22	53,53,53,53	0
58	MG	1A	3129	1/1	0.88	0.20	47,47,47,47	0
58	MG	1A	3759	1/1	0.88	0.24	44,44,44,44	0
58	MG	2A	3253	1/1	0.88	0.15	70,70,70,70	0
58	MG	1A	3483	1/1	0.88	0.16	69,69,69,69	0
58	MG	2B	201	1/1	0.88	0.13	79,79,79,79	0
58	MG	2B	203	1/1	0.88	0.07	77,77,77,77	0
58	MG	2A	3159	1/1	0.88	0.29	70,70,70,70	0
58	MG	2a	1695	1/1	0.88	0.09	63,63,63,63	0
58	MG	2A	3043	1/1	0.88	0.34	69,69,69,69	0
58	MG	1A	3184	1/1	0.88	0.17	50,50,50,50	0
58	MG	1A	3630	1/1	0.88	0.23	38,38,38,38	0
58	MG	1a	1761	1/1	0.88	0.14	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1E	315	1/1	0.88	0.05	46,46,46,46	0
58	MG	2A	3592	1/1	0.88	0.13	69,69,69,69	0
58	MG	1A	3359	1/1	0.88	0.14	65,65,65,65	0
58	MG	1A	3643	1/1	0.88	0.20	31,31,31,31	0
58	MG	1A	3544	1/1	0.88	0.14	47,47,47,47	0
58	MG	2E	304	1/1	0.88	0.25	57,57,57,57	0
58	MG	2A	3061	1/1	0.88	0.21	70,70,70,70	0
58	MG	2A	3385	1/1	0.88	0.26	61,61,61,61	0
58	MG	1A	3269	1/1	0.88	0.21	60,60,60,60	0
58	MG	1A	3493	1/1	0.88	0.17	60,60,60,60	0
58	MG	1a	1652	1/1	0.88	0.31	83,83,83,83	0
58	MG	1A	3652	1/1	0.88	0.20	37,37,37,37	0
58	MG	2a	1727	1/1	0.88	0.11	84,84,84,84	0
58	MG	2a	1731	1/1	0.88	0.17	64,64,64,64	0
58	MG	2O	201	1/1	0.88	0.15	67,67,67,67	0
58	MG	2A	3390	1/1	0.88	0.48	73,73,73,73	0
58	MG	1A	3796	1/1	0.88	0.09	78,78,78,78	0
58	MG	2a	1737	1/1	0.88	0.06	77,77,77,77	0
58	MG	2a	1742	1/1	0.88	0.19	103,103,103,103	0
58	MG	1A	3653	1/1	0.88	0.12	41,41,41,41	0
58	MG	1A	3927	1/1	0.88	0.18	68,68,68,68	0
58	MG	1A	3131	1/1	0.88	0.48	52,52,52,52	0
58	MG	1a	1665	1/1	0.88	0.17	69,69,69,69	0
58	MG	1A	3419	1/1	0.88	0.24	66,66,66,66	0
58	MG	2a	1757	1/1	0.88	0.08	92,92,92,92	0
58	MG	1A	3672	1/1	0.88	0.25	37,37,37,37	0
58	MG	1A	3810	1/1	0.88	0.13	56,56,56,56	0
58	MG	1A	3499	1/1	0.88	0.15	73,73,73,73	0
58	MG	1A	3006	1/1	0.88	0.18	69,69,69,69	0
58	MG	2a	1765	1/1	0.88	0.15	82,82,82,82	0
58	MG	2a	1777	1/1	0.88	0.27	68,68,68,68	0
58	MG	1A	3565	1/1	0.88	0.31	43,43,43,43	0
58	MG	1A	3566	1/1	0.88	0.31	50,50,50,50	0
58	MG	1A	3952	1/1	0.88	0.22	55,55,55,55	0
58	MG	1A	3301	1/1	0.88	0.37	57,57,57,57	0
58	MG	1A	3573	1/1	0.88	0.21	49,49,49,49	0
58	MG	1A	3343	1/1	0.88	0.51	57,57,57,57	0
58	MG	2A	3435	1/1	0.88	0.30	61,61,61,61	0
58	MG	2A	3314	1/1	0.88	0.12	79,79,79,79	0
58	MG	10	108	1/1	0.88	0.13	54,54,54,54	0
58	MG	2A	3448	1/1	0.88	0.17	52,52,52,52	0
58	MG	1A	3393	1/1	0.88	0.50	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	12	101	1/1	0.88	0.18	66,66,66,66	0
58	MG	1A	3706	1/1	0.88	0.16	56,56,56,56	0
58	MG	1A	3320	1/1	0.88	0.19	48,48,48,48	0
58	MG	15	107	1/1	0.88	0.25	54,54,54,54	0
58	MG	2a	1813	1/1	0.88	0.14	95,95,95,95	0
58	MG	1A	3016	1/1	0.88	0.34	53,53,53,53	0
58	MG	1A	3349	1/1	0.88	0.29	68,68,68,68	0
58	MG	2a	1623	1/1	0.88	0.43	83,83,83,83	0
58	MG	2A	3713	1/1	0.88	0.18	56,56,56,56	0
58	MG	2A	3492	1/1	0.88	0.12	61,61,61,61	0
58	MG	2A	3497	1/1	0.88	0.16	54,54,54,54	0
58	MG	1A	3398	1/1	0.88	0.52	47,47,47,47	0
58	MG	1A	3845	1/1	0.88	0.17	73,73,73,73	0
58	MG	1a	1707	1/1	0.88	0.26	72,72,72,72	0
58	MG	1A	3729	1/1	0.88	0.14	64,64,64,64	0
58	MG	1A	3989	1/1	0.88	0.09	55,55,55,55	0
58	MG	2A	3738	1/1	0.88	0.17	81,81,81,81	0
58	MG	1B	207	1/1	0.88	0.15	75,75,75,75	0
58	MG	2A	3338	1/1	0.88	0.24	67,67,67,67	0
58	MG	1A	3847	1/1	0.88	0.19	55,55,55,55	0
58	MG	2A	3007	1/1	0.88	0.07	59,59,59,59	0
58	MG	1A	3441	1/1	0.88	0.32	60,60,60,60	0
58	MG	1B	213	1/1	0.88	0.08	71,71,71,71	0
58	MG	1A	3477	1/1	0.88	0.29	47,47,47,47	0
58	MG	2A	3553	1/1	0.88	0.34	52,52,52,52	0
58	MG	1A	3171	1/1	0.88	0.15	57,57,57,57	0
58	MG	1A	3205	1/1	0.89	0.16	70,70,70,70	0
58	MG	2A	3402	1/1	0.89	0.26	71,71,71,71	0
58	MG	1A	3322	1/1	0.89	0.18	59,59,59,59	0
58	MG	1a	1663	1/1	0.89	0.09	86,86,86,86	0
58	MG	1U	205	1/1	0.89	0.35	44,44,44,44	0
58	MG	1A	3226	1/1	0.89	0.20	56,56,56,56	0
58	MG	1A	3680	1/1	0.89	0.27	36,36,36,36	0
58	MG	1a	1793	1/1	0.89	0.15	83,83,83,83	0
58	MG	2A	3689	1/1	0.89	0.18	80,80,80,80	0
58	MG	1A	4080	1/1	0.89	0.14	49,49,49,49	0
58	MG	1A	3432	1/1	0.89	0.14	56,56,56,56	0
58	MG	1A	3908	1/1	0.89	0.14	62,62,62,62	0
58	MG	2A	3068	1/1	0.89	0.28	62,62,62,62	0
58	MG	2A	3191	1/1	0.89	0.14	78,78,78,78	0
58	MG	2A	3072	1/1	0.89	0.33	70,70,70,70	0
58	MG	1a	1807	1/1	0.89	0.21	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3305	1/1	0.89	0.22	68,68,68,68	0
58	MG	1A	3517	1/1	0.89	0.20	58,58,58,58	0
58	MG	2A	3453	1/1	0.89	0.15	66,66,66,66	0
58	MG	2a	1664	1/1	0.89	0.24	75,75,75,75	0
58	MG	2A	3723	1/1	0.89	0.16	61,61,61,61	0
58	MG	1a	1811	1/1	0.89	0.11	70,70,70,70	0
58	MG	2A	3459	1/1	0.89	0.18	81,81,81,81	0
58	MG	2A	3732	1/1	0.89	0.23	78,78,78,78	0
58	MG	2A	3462	1/1	0.89	0.15	50,50,50,50	0
58	MG	2A	3198	1/1	0.89	0.23	66,66,66,66	0
58	MG	1A	3576	1/1	0.89	0.15	65,65,65,65	0
58	MG	2A	3739	1/1	0.89	0.12	89,89,89,89	0
58	MG	2A	3474	1/1	0.89	0.28	42,42,42,42	0
58	MG	2a	1687	1/1	0.89	0.22	57,57,57,57	0
58	MG	2A	3081	1/1	0.89	0.12	69,69,69,69	0
58	MG	2A	3484	1/1	0.89	0.18	53,53,53,53	0
58	MG	2A	3748	1/1	0.89	0.14	55,55,55,55	0
58	MG	2A	3082	1/1	0.89	0.20	61,61,61,61	0
58	MG	1B	211	1/1	0.89	0.22	58,58,58,58	0
58	MG	1A	3274	1/1	0.89	0.32	57,57,57,57	0
58	MG	1A	3080	1/1	0.89	0.18	48,48,48,48	0
58	MG	1A	3438	1/1	0.89	0.27	69,69,69,69	0
58	MG	2A	3321	1/1	0.89	0.32	58,58,58,58	0
58	MG	2A	3503	1/1	0.89	0.36	68,68,68,68	0
58	MG	1A	3522	1/1	0.89	0.28	61,61,61,61	0
58	MG	2A	3209	1/1	0.89	0.30	74,74,74,74	0
58	MG	1n	102	1/1	0.89	0.17	74,74,74,74	0
58	MG	1A	3185	1/1	0.89	0.13	55,55,55,55	0
58	MG	1A	3586	1/1	0.89	0.19	40,40,40,40	0
58	MG	2A	3331	1/1	0.89	0.37	71,71,71,71	0
58	MG	2A	3531	1/1	0.89	0.26	43,43,43,43	0
58	MG	1A	3355	1/1	0.89	0.15	69,69,69,69	0
58	MG	1A	3823	1/1	0.89	0.22	45,45,45,45	0
58	MG	2A	3535	1/1	0.89	0.30	54,54,54,54	0
58	MG	2a	1728	1/1	0.89	0.23	92,92,92,92	0
58	MG	1A	3068	1/1	0.89	0.25	35,35,35,35	0
58	MG	1B	235	1/1	0.89	0.24	79,79,79,79	0
58	MG	1A	3380	1/1	0.89	0.16	47,47,47,47	0
58	MG	1a	1606	1/1	0.89	0.17	65,65,65,65	0
58	MG	2A	3560	1/1	0.89	0.28	51,51,51,51	0
58	MG	2a	1738	1/1	0.89	0.15	75,75,75,75	0
58	MG	1A	3941	1/1	0.89	0.16	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	1D	3608	1/1	0.89	0.31	59,59,59,59	0
58	MG	1A	3237	1/1	0.89	0.34	60,60,60,60	0
58	MG	1A	3040	1/1	0.89	0.16	45,45,45,45	0
58	MG	1E	310	1/1	0.89	0.22	29,29,29,29	0
58	MG	1A	3413	1/1	0.89	0.22	53,53,53,53	0
58	MG	1A	3744	1/1	0.89	0.23	30,30,30,30	0
58	MG	1A	3488	1/1	0.89	0.37	56,56,56,56	0
58	MG	1A	3051	1/1	0.89	0.48	55,55,55,55	0
58	MG	2A	3353	1/1	0.89	0.35	53,53,53,53	0
58	MG	2A	3578	1/1	0.89	0.29	73,73,73,73	0
58	MG	2A	3355	1/1	0.89	0.31	66,66,66,66	0
58	MG	1A	3542	1/1	0.89	0.17	62,62,62,62	0
58	MG	1A	3631	1/1	0.89	0.08	41,41,41,41	0
58	MG	1A	3492	1/1	0.89	0.20	38,38,38,38	0
58	MG	1a	1722	1/1	0.89	0.22	51,51,51,51	0
58	MG	2A	3131	1/1	0.89	0.18	68,68,68,68	0
58	MG	1I	201	1/1	0.89	0.22	73,73,73,73	0
58	MG	2A	3010	1/1	0.89	0.16	73,73,73,73	0
58	MG	2A	3136	1/1	0.89	0.28	69,69,69,69	0
58	MG	1A	3418	1/1	0.89	0.20	62,62,62,62	0
58	MG	2A	3601	1/1	0.89	0.20	68,68,68,68	0
58	MG	1A	3555	1/1	0.89	0.30	48,48,48,48	0
58	MG	2A	3375	1/1	0.89	0.50	70,70,70,70	0
58	MG	2a	1803	1/1	0.89	0.08	72,72,72,72	0
58	MG	1a	1640	1/1	0.89	0.21	76,76,76,76	0
58	MG	1O	206	1/1	0.89	0.24	74,74,74,74	0
58	MG	2A	3143	1/1	0.89	0.30	49,49,49,49	0
58	MG	2a	1811	1/1	0.89	0.20	76,76,76,76	0
58	MG	2A	3614	1/1	0.89	0.11	88,88,88,88	0
58	MG	2A	3024	1/1	0.89	0.23	72,72,72,72	0
58	MG	1A	3337	1/1	0.89	0.32	60,60,60,60	0
58	MG	2A	3256	1/1	0.89	0.26	80,80,80,80	0
58	MG	2A	3629	1/1	0.89	0.19	75,75,75,75	0
58	MG	1A	3771	1/1	0.89	0.09	54,54,54,54	0
58	MG	2A	3636	1/1	0.89	0.19	71,71,71,71	0
58	MG	1A	3264	1/1	0.89	0.12	63,63,63,63	0
58	MG	2A	3641	1/1	0.89	0.23	64,64,64,64	0
58	MG	1A	3089	1/1	0.89	0.31	52,52,52,52	0
58	MG	2a	1611	1/1	0.89	0.18	74,74,74,74	0
58	MG	2a	1612	1/1	0.89	0.11	74,74,74,74	0
58	MG	1R	205	1/1	0.89	0.38	54,54,54,54	0
58	MG	2A	3038	1/1	0.89	0.16	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	1764	1/1	0.89	0.21	75,75,75,75	0
58	MG	1a	1765	1/1	0.89	0.17	84,84,84,84	0
58	MG	1A	3501	1/1	0.89	0.20	56,56,56,56	0
58	MG	2A	3163	1/1	0.89	0.14	75,75,75,75	0
58	MG	1S	201	1/1	0.89	0.34	55,55,55,55	0
58	MG	2A	3399	1/1	0.89	0.23	69,69,69,69	0
58	MG	2A	3666	1/1	0.89	0.10	72,72,72,72	0
58	MG	2A	3667	1/1	0.89	0.43	50,50,50,50	0
58	MG	1A	3183	1/1	0.89	0.09	79,79,79,79	0
61	ZN	29	501	1/1	0.89	0.09	83,83,83,83	0
58	MG	1a	1778	1/1	0.90	0.20	84,84,84,84	0
58	MG	1a	1650	1/1	0.90	0.12	67,67,67,67	0
58	MG	1A	3841	1/1	0.90	0.10	65,65,65,65	0
58	MG	2A	3062	1/1	0.90	0.15	60,60,60,60	0
58	MG	2A	3660	1/1	0.90	0.22	73,73,73,73	0
58	MG	2A	3412	1/1	0.90	0.26	69,69,69,69	0
58	MG	1A	3842	1/1	0.90	0.31	44,44,44,44	0
58	MG	1A	3487	1/1	0.90	0.22	58,58,58,58	0
58	MG	2A	3416	1/1	0.90	0.13	90,90,90,90	0
58	MG	1A	3111	1/1	0.90	0.21	47,47,47,47	0
58	MG	2A	3670	1/1	0.90	0.21	85,85,85,85	0
58	MG	2A	3296	1/1	0.90	0.22	72,72,72,72	0
58	MG	1A	3198	1/1	0.90	0.20	55,55,55,55	0
58	MG	2A	3299	1/1	0.90	0.23	68,68,68,68	0
58	MG	1a	1796	1/1	0.90	0.19	77,77,77,77	0
58	MG	2A	3683	1/1	0.90	0.32	62,62,62,62	0
58	MG	2A	3304	1/1	0.90	0.26	62,62,62,62	0
58	MG	1A	3668	1/1	0.90	0.21	80,80,80,80	0
58	MG	1A	3376	1/1	0.90	0.36	67,67,67,67	0
58	MG	1A	3401	1/1	0.90	0.13	46,46,46,46	0
58	MG	2A	3308	1/1	0.90	0.20	63,63,63,63	0
58	MG	1U	204	1/1	0.90	0.24	45,45,45,45	0
58	MG	2A	3694	1/1	0.90	0.19	76,76,76,76	0
58	MG	2A	3458	1/1	0.90	0.16	52,52,52,52	0
58	MG	1A	3494	1/1	0.90	0.58	56,56,56,56	0
58	MG	2A	3460	1/1	0.90	0.22	38,38,38,38	0
58	MG	2A	3702	1/1	0.90	0.53	86,86,86,86	0
58	MG	1a	1670	1/1	0.90	0.30	75,75,75,75	0
58	MG	1A	3976	1/1	0.90	0.20	41,41,41,41	0
58	MG	1A	3978	1/1	0.90	0.23	27,27,27,27	0
58	MG	1A	3142	1/1	0.90	0.14	58,58,58,58	0
58	MG	2A	3475	1/1	0.90	0.23	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	2a	1670	1/1	0.90	0.13	84,84,84,84	0
58	MG	2A	3476	1/1	0.90	0.13	66,66,66,66	0
58	MG	2A	3479	1/1	0.90	0.17	71,71,71,71	0
58	MG	2a	1675	1/1	0.90	0.12	81,81,81,81	0
58	MG	1A	3982	1/1	0.90	0.06	59,59,59,59	0
58	MG	1A	3379	1/1	0.90	0.40	42,42,42,42	0
58	MG	1Z	303	1/1	0.90	0.18	74,74,74,74	0
58	MG	10	103	1/1	0.90	0.16	57,57,57,57	0
58	MG	1A	4081	1/1	0.90	0.22	50,50,50,50	0
58	MG	2A	3496	1/1	0.90	0.16	59,59,59,59	0
58	MG	10	106	1/1	0.90	0.10	59,59,59,59	0
58	MG	1A	3870	1/1	0.90	0.19	39,39,39,39	0
58	MG	1a	1689	1/1	0.90	0.07	74,74,74,74	0
58	MG	2A	3500	1/1	0.90	0.23	37,37,37,37	0
58	MG	1A	3085	1/1	0.90	0.44	42,42,42,42	0
58	MG	2A	3512	1/1	0.90	0.11	57,57,57,57	0
58	MG	2A	3754	1/1	0.90	0.27	44,44,44,44	0
58	MG	2A	3755	1/1	0.90	0.12	61,61,61,61	0
58	MG	1A	3791	1/1	0.90	0.14	67,67,67,67	0
58	MG	2A	3333	1/1	0.90	0.25	76,76,76,76	0
58	MG	2A	3760	1/1	0.90	0.06	60,60,60,60	0
58	MG	2A	3761	1/1	0.90	0.23	48,48,48,48	0
58	MG	2A	3334	1/1	0.90	0.11	86,86,86,86	0
58	MG	2A	3768	1/1	0.90	0.12	76,76,76,76	0
58	MG	1A	3882	1/1	0.90	0.16	51,51,51,51	0
58	MG	2a	1713	1/1	0.90	0.20	70,70,70,70	0
58	MG	1A	3020	1/1	0.90	0.21	64,64,64,64	0
58	MG	1A	3794	1/1	0.90	0.22	59,59,59,59	0
58	MG	2a	1718	1/1	0.90	0.10	80,80,80,80	0
58	MG	2a	1720	1/1	0.90	0.16	77,77,77,77	0
58	MG	1a	1696	1/1	0.90	0.45	69,69,69,69	0
58	MG	2a	1725	1/1	0.90	0.28	80,80,80,80	0
58	MG	2a	1726	1/1	0.90	0.14	88,88,88,88	0
58	MG	1A	3070	1/1	0.90	0.15	36,36,36,36	0
58	MG	1A	3890	1/1	0.90	0.31	64,64,64,64	0
58	MG	1A	4003	1/1	0.90	0.17	27,27,27,27	0
58	MG	1A	3692	1/1	0.90	0.08	69,69,69,69	0
58	MG	2A	3540	1/1	0.90	0.18	80,80,80,80	0
58	MG	2A	3788	1/1	0.90	0.21	63,63,63,63	0
58	MG	2A	3792	1/1	0.90	0.31	63,63,63,63	0
58	MG	2A	3544	1/1	0.90	0.27	64,64,64,64	0
58	MG	1A	3693	1/1	0.90	0.15	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	1x	109	1/1	0.90	0.36	84,84,84,84	0
58	MG	1A	3545	1/1	0.90	0.10	77,77,77,77	0
58	MG	1A	3614	1/1	0.90	0.17	41,41,41,41	0
58	MG	1A	4016	1/1	0.90	0.12	78,78,78,78	0
58	MG	1A	3310	1/1	0.90	0.31	67,67,67,67	0
58	MG	1a	1613	1/1	0.90	0.07	79,79,79,79	0
58	MG	2A	3354	1/1	0.90	0.34	66,66,66,66	0
58	MG	1D	3601	1/1	0.90	0.35	54,54,54,54	0
58	MG	1A	3511	1/1	0.90	0.74	53,53,53,53	0
58	MG	2A	3360	1/1	0.90	0.58	70,70,70,70	0
58	MG	1A	3444	1/1	0.90	0.20	49,49,49,49	0
58	MG	2a	1776	1/1	0.90	0.17	69,69,69,69	0
58	MG	2A	3014	1/1	0.90	0.19	45,45,45,45	0
58	MG	1a	1719	1/1	0.90	0.25	72,72,72,72	0
58	MG	2B	218	1/1	0.90	0.30	78,78,78,78	0
58	MG	1A	3914	1/1	0.90	0.18	65,65,65,65	0
58	MG	2a	1783	1/1	0.90	0.11	77,77,77,77	0
58	MG	2A	3366	1/1	0.90	0.43	70,70,70,70	0
58	MG	1A	4028	1/1	0.90	0.20	78,78,78,78	0
58	MG	2A	3141	1/1	0.90	0.16	78,78,78,78	0
58	MG	2A	3584	1/1	0.90	0.16	46,46,46,46	0
58	MG	1A	3046	1/1	0.90	0.15	38,38,38,38	0
58	MG	1A	3515	1/1	0.90	0.27	69,69,69,69	0
58	MG	2a	1800	1/1	0.90	0.28	80,80,80,80	0
58	MG	2A	3587	1/1	0.90	0.24	77,77,77,77	0
58	MG	2A	3588	1/1	0.90	0.13	81,81,81,81	0
58	MG	1A	3918	1/1	0.90	0.10	47,47,47,47	0
58	MG	2a	1804	1/1	0.90	0.32	75,75,75,75	0
58	MG	2Q	202	1/1	0.90	0.33	68,68,68,68	0
58	MG	1A	3170	1/1	0.90	0.21	59,59,59,59	0
58	MG	1A	3389	1/1	0.90	0.29	44,44,44,44	0
58	MG	1A	3635	1/1	0.90	0.09	51,51,51,51	0
58	MG	1A	3636	1/1	0.90	0.23	53,53,53,53	0
58	MG	2X	101	1/1	0.90	0.14	60,60,60,60	0
58	MG	2A	3380	1/1	0.90	0.42	66,66,66,66	0
58	MG	1A	3740	1/1	0.90	0.21	60,60,60,60	0
58	MG	1A	3935	1/1	0.90	0.16	55,55,55,55	0
58	MG	1A	3188	1/1	0.90	0.42	47,47,47,47	0
58	MG	2a	1821	1/1	0.90	0.08	76,76,76,76	0
58	MG	2A	3160	1/1	0.90	0.15	57,57,57,57	0
58	MG	1A	3938	1/1	0.90	0.20	61,61,61,61	0
58	MG	2A	3045	1/1	0.90	0.14	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	27	102	1/1	0.90	0.34	68,68,68,68	0
58	MG	2A	3046	1/1	0.90	0.10	75,75,75,75	0
58	MG	1N	204	1/1	0.90	0.26	52,52,52,52	0
58	MG	2A	3625	1/1	0.90	0.10	58,58,58,58	0
58	MG	2A	3165	1/1	0.90	0.19	76,76,76,76	0
58	MG	2A	3274	1/1	0.90	0.21	80,80,80,80	0
58	MG	1A	3645	1/1	0.90	0.17	30,30,30,30	0
58	MG	2A	3276	1/1	0.90	0.30	67,67,67,67	0
58	MG	2A	3277	1/1	0.90	0.50	65,65,65,65	0
58	MG	1A	3090	1/1	0.90	0.30	62,62,62,62	0
58	MG	2A	3642	1/1	0.90	0.13	80,80,80,80	0
58	MG	1A	3394	1/1	0.90	0.19	65,65,65,65	0
58	MG	2A	3644	1/1	0.90	0.17	54,54,54,54	0
59	K	1A	3559	1/1	0.90	0.12	81,81,81,81	0
58	MG	1A	3221	1/1	0.90	0.15	59,59,59,59	0
58	MG	2A	3057	1/1	0.90	0.15	78,78,78,78	0
58	MG	2A	3180	1/1	0.91	0.09	66,66,66,66	0
58	MG	1O	202	1/1	0.91	0.39	56,56,56,56	0
58	MG	1A	4027	1/1	0.91	0.09	52,52,52,52	0
58	MG	20	103	1/1	0.91	0.24	76,76,76,76	0
58	MG	1a	1683	1/1	0.91	0.36	70,70,70,70	0
58	MG	2A	3582	1/1	0.91	0.18	68,68,68,68	0
58	MG	2A	3015	1/1	0.91	0.19	58,58,58,58	0
58	MG	2A	3016	1/1	0.91	0.32	87,87,87,87	0
58	MG	27	101	1/1	0.91	0.26	48,48,48,48	0
58	MG	1A	3891	1/1	0.91	0.17	62,62,62,62	0
58	MG	1a	1686	1/1	0.91	0.19	69,69,69,69	0
58	MG	1A	3892	1/1	0.91	0.17	45,45,45,45	0
58	MG	1A	3455	1/1	0.91	0.27	74,74,74,74	0
58	MG	1A	3210	1/1	0.91	0.40	57,57,57,57	0
58	MG	1A	3901	1/1	0.91	0.21	37,37,37,37	0
58	MG	2A	3594	1/1	0.91	0.46	79,79,79,79	0
58	MG	1A	3638	1/1	0.91	0.21	44,44,44,44	0
58	MG	1A	3553	1/1	0.91	0.65	56,56,56,56	0
58	MG	2a	1607	1/1	0.91	0.10	77,77,77,77	0
58	MG	1A	3910	1/1	0.91	0.12	53,53,53,53	0
58	MG	2A	3036	1/1	0.91	0.20	41,41,41,41	0
58	MG	1A	3058	1/1	0.91	0.27	66,66,66,66	0
58	MG	1A	3500	1/1	0.91	0.18	49,49,49,49	0
58	MG	1A	3647	1/1	0.91	0.14	46,46,46,46	0
58	MG	1a	1701	1/1	0.91	0.36	63,63,63,63	0
58	MG	2a	1615	1/1	0.91	0.14	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3390	1/1	0.91	0.30	49,49,49,49	0
58	MG	2A	3617	1/1	0.91	0.07	69,69,69,69	0
58	MG	1A	3121	1/1	0.91	0.32	51,51,51,51	0
58	MG	1A	3504	1/1	0.91	0.16	65,65,65,65	0
58	MG	2A	3623	1/1	0.91	0.07	78,78,78,78	0
58	MG	1A	3917	1/1	0.91	0.19	44,44,44,44	0
58	MG	1A	3462	1/1	0.91	0.19	65,65,65,65	0
58	MG	1W	202	1/1	0.91	0.34	58,58,58,58	0
58	MG	2A	3630	1/1	0.91	0.08	72,72,72,72	0
58	MG	2A	3369	1/1	0.91	0.20	65,65,65,65	0
58	MG	1A	3507	1/1	0.91	0.24	78,78,78,78	0
58	MG	2a	1632	1/1	0.91	0.17	87,87,87,87	0
58	MG	2A	3637	1/1	0.91	0.17	67,67,67,67	0
58	MG	1a	1711	1/1	0.91	0.16	59,59,59,59	0
58	MG	1A	3463	1/1	0.91	0.35	46,46,46,46	0
58	MG	1A	3465	1/1	0.91	0.20	61,61,61,61	0
58	MG	1A	3338	1/1	0.91	0.22	62,62,62,62	0
58	MG	2a	1639	1/1	0.91	0.42	74,74,74,74	0
58	MG	2A	3060	1/1	0.91	0.24	58,58,58,58	0
58	MG	2A	3647	1/1	0.91	0.25	55,55,55,55	0
58	MG	2A	3222	1/1	0.91	0.42	70,70,70,70	0
58	MG	2a	1646	1/1	0.91	0.07	84,84,84,84	0
58	MG	1A	3674	1/1	0.91	0.19	39,39,39,39	0
58	MG	1A	3675	1/1	0.91	0.11	78,78,78,78	0
58	MG	1A	4062	1/1	0.91	0.13	44,44,44,44	0
58	MG	2a	1652	1/1	0.91	0.18	84,84,84,84	0
58	MG	1a	1720	1/1	0.91	0.11	53,53,53,53	0
58	MG	1l	104	1/1	0.91	0.15	78,78,78,78	0
58	MG	1A	3234	1/1	0.91	0.18	67,67,67,67	0
58	MG	2A	3661	1/1	0.91	0.21	77,77,77,77	0
58	MG	1a	1723	1/1	0.91	0.39	66,66,66,66	0
58	MG	2A	3069	1/1	0.91	0.21	35,35,35,35	0
58	MG	2A	3071	1/1	0.91	0.17	64,64,64,64	0
58	MG	1A	3341	1/1	0.91	0.25	64,64,64,64	0
58	MG	1A	3367	1/1	0.91	0.15	68,68,68,68	0
58	MG	15	106	1/1	0.91	0.17	41,41,41,41	0
58	MG	2A	3238	1/1	0.91	0.30	60,60,60,60	0
58	MG	2A	3676	1/1	0.91	0.20	65,65,65,65	0
58	MG	1A	3686	1/1	0.91	0.15	65,65,65,65	0
58	MG	1A	3579	1/1	0.91	0.19	47,47,47,47	0
58	MG	1A	4074	1/1	0.91	0.17	39,39,39,39	0
58	MG	1A	3071	1/1	0.91	0.49	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3581	1/1	0.91	0.44	58,58,58,58	0
58	MG	2a	1682	1/1	0.91	0.18	84,84,84,84	0
58	MG	1a	1751	1/1	0.91	0.28	81,81,81,81	0
58	MG	2A	3248	1/1	0.91	0.20	83,83,83,83	0
58	MG	1A	3244	1/1	0.91	0.37	66,66,66,66	0
58	MG	1A	3824	1/1	0.91	0.26	71,71,71,71	0
58	MG	2a	1691	1/1	0.91	0.32	83,83,83,83	0
58	MG	2A	3411	1/1	0.91	0.13	63,63,63,63	0
58	MG	1a	1604	1/1	0.91	0.10	71,71,71,71	0
58	MG	2A	3696	1/1	0.91	0.21	87,87,87,87	0
58	MG	2A	3089	1/1	0.91	0.24	72,72,72,72	0
58	MG	1A	4086	1/1	0.91	0.22	66,66,66,66	0
58	MG	2A	3415	1/1	0.91	0.21	72,72,72,72	0
58	MG	2A	3092	1/1	0.91	0.29	59,59,59,59	0
58	MG	2A	3417	1/1	0.91	0.33	63,63,63,63	0
58	MG	1A	3954	1/1	0.91	0.19	33,33,33,33	0
58	MG	2A	3709	1/1	0.91	0.19	83,83,83,83	0
58	MG	1A	3092	1/1	0.91	0.18	32,32,32,32	0
58	MG	1a	1609	1/1	0.91	0.27	62,62,62,62	0
58	MG	1a	1776	1/1	0.91	0.14	78,78,78,78	0
58	MG	2A	3430	1/1	0.91	0.08	89,89,89,89	0
58	MG	1a	1611	1/1	0.91	0.18	39,39,39,39	0
58	MG	2A	3729	1/1	0.91	0.12	72,72,72,72	0
58	MG	1A	3220	1/1	0.91	0.17	54,54,54,54	0
58	MG	2A	3443	1/1	0.91	0.14	53,53,53,53	0
58	MG	2A	3444	1/1	0.91	0.14	75,75,75,75	0
58	MG	1A	3698	1/1	0.91	0.14	59,59,59,59	0
58	MG	1A	3700	1/1	0.91	0.13	67,67,67,67	0
58	MG	2A	3449	1/1	0.91	0.22	50,50,50,50	0
58	MG	1A	3321	1/1	0.91	0.40	43,43,43,43	0
58	MG	2A	3741	1/1	0.91	0.21	78,78,78,78	0
58	MG	2A	3110	1/1	0.91	0.19	83,83,83,83	0
58	MG	2A	3271	1/1	0.91	0.14	73,73,73,73	0
58	MG	1A	3971	1/1	0.91	0.10	81,81,81,81	0
58	MG	1A	3526	1/1	0.91	0.44	47,47,47,47	0
58	MG	1a	1621	1/1	0.91	0.09	50,50,50,50	0
58	MG	2A	3753	1/1	0.91	0.30	52,52,52,52	0
58	MG	1A	3974	1/1	0.91	0.07	52,52,52,52	0
58	MG	2a	1746	1/1	0.91	0.11	85,85,85,85	0
58	MG	2a	1748	1/1	0.91	0.11	94,94,94,94	0
58	MG	1A	3591	1/1	0.91	0.12	69,69,69,69	0
58	MG	1a	1801	1/1	0.91	0.26	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	2A	3468	1/1	0.91	0.22	58,58,58,58	0
58	MG	2A	3759	1/1	0.91	0.32	60,60,60,60	0
58	MG	2A	3473	1/1	0.91	0.22	54,54,54,54	0
58	MG	1A	3405	1/1	0.91	0.14	59,59,59,59	0
58	MG	2A	3763	1/1	0.91	0.29	70,70,70,70	0
58	MG	1A	3596	1/1	0.91	0.16	59,59,59,59	0
58	MG	1A	3597	1/1	0.91	0.20	35,35,35,35	0
58	MG	2a	1762	1/1	0.91	0.14	74,74,74,74	0
58	MG	1B	232	1/1	0.91	0.12	79,79,79,79	0
58	MG	1A	3721	1/1	0.91	0.16	51,51,51,51	0
58	MG	1A	3605	1/1	0.91	0.20	38,38,38,38	0
58	MG	1A	3445	1/1	0.91	0.33	46,46,46,46	0
58	MG	1A	3247	1/1	0.91	0.26	80,80,80,80	0
58	MG	1A	3860	1/1	0.91	0.32	46,46,46,46	0
58	MG	1l	202	1/1	0.91	0.17	76,76,76,76	0
58	MG	1A	3734	1/1	0.91	0.15	46,46,46,46	0
58	MG	2A	3295	1/1	0.91	0.14	83,83,83,83	0
58	MG	1A	3145	1/1	0.91	0.47	38,38,38,38	0
58	MG	2A	3790	1/1	0.91	0.18	55,55,55,55	0
58	MG	1E	303	1/1	0.91	0.30	52,52,52,52	0
58	MG	2A	3298	1/1	0.91	0.29	69,69,69,69	0
58	MG	1a	1646	1/1	0.91	0.29	66,66,66,66	0
58	MG	2A	3301	1/1	0.91	0.17	76,76,76,76	0
58	MG	1A	3739	1/1	0.91	0.18	56,56,56,56	0
58	MG	1A	3324	1/1	0.91	0.14	59,59,59,59	0
58	MG	1E	311	1/1	0.91	0.23	32,32,32,32	0
58	MG	2A	3526	1/1	0.91	0.17	67,67,67,67	0
58	MG	1A	3018	1/1	0.91	0.23	45,45,45,45	0
58	MG	2A	3151	1/1	0.91	0.32	58,58,58,58	0
58	MG	1A	3747	1/1	0.91	0.17	52,52,52,52	0
58	MG	2A	3154	1/1	0.91	0.24	71,71,71,71	0
58	MG	1F	303	1/1	0.91	0.15	45,45,45,45	0
58	MG	1a	1657	1/1	0.91	0.16	62,62,62,62	0
58	MG	1F	305	1/1	0.91	0.16	39,39,39,39	0
58	MG	2B	214	1/1	0.91	0.17	81,81,81,81	0
58	MG	1A	3874	1/1	0.91	0.21	31,31,31,31	0
58	MG	1A	4006	1/1	0.91	0.18	34,34,34,34	0
58	MG	2D	301	1/1	0.91	0.29	58,58,58,58	0
58	MG	1A	3306	1/1	0.91	0.45	68,68,68,68	0
58	MG	2A	3551	1/1	0.91	0.14	75,75,75,75	0
58	MG	2E	303	1/1	0.91	0.15	68,68,68,68	0
58	MG	1G	202	1/1	0.91	0.32	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3540	1/1	0.91	0.31	69,69,69,69	0
58	MG	1A	3273	1/1	0.91	0.10	54,54,54,54	0
58	MG	2I	201	1/1	0.91	0.12	84,84,84,84	0
58	MG	1A	3757	1/1	0.91	0.11	42,42,42,42	0
58	MG	1a	1671	1/1	0.91	0.08	77,77,77,77	0
58	MG	1N	201	1/1	0.91	0.34	50,50,50,50	0
58	MG	2t	201	1/1	0.91	0.09	62,62,62,62	0
58	MG	2F	307	1/1	0.91	0.37	57,57,57,57	0
58	MG	1A	3150	1/1	0.91	0.59	50,50,50,50	0
58	MG	2A	3329	1/1	0.91	0.21	66,66,66,66	0
58	MG	2A	3330	1/1	0.91	0.21	77,77,77,77	0
58	MG	1A	3888	1/1	0.91	0.16	49,49,49,49	0
58	MG	1A	3094	1/1	0.91	0.20	64,64,64,64	0
58	MG	2A	3175	1/1	0.91	0.20	61,61,61,61	0
58	MG	2U	201	1/1	0.91	0.59	70,70,70,70	0
58	MG	1O	201	1/1	0.91	0.36	65,65,65,65	0
58	MG	2A	3577	1/1	0.91	0.17	84,84,84,84	0
61	ZN	2n	501	1/1	0.91	0.08	117,117,117,117	0
58	MG	1A	3204	1/1	0.92	0.14	44,44,44,44	0
58	MG	1A	3682	1/1	0.92	0.11	63,63,63,63	0
58	MG	1A	3332	1/1	0.92	0.06	65,65,65,65	0
58	MG	2A	3117	1/1	0.92	0.29	59,59,59,59	0
58	MG	2A	3658	1/1	0.92	0.13	68,68,68,68	0
58	MG	1A	3373	1/1	0.92	0.47	56,56,56,56	0
58	MG	1e	201	1/1	0.92	0.43	73,73,73,73	0
58	MG	1e	203	1/1	0.92	0.56	74,74,74,74	0
58	MG	1a	1654	1/1	0.92	0.20	52,52,52,52	0
58	MG	2A	3422	1/1	0.92	0.26	74,74,74,74	0
58	MG	1A	3114	1/1	0.92	0.51	53,53,53,53	0
58	MG	1N	203	1/1	0.92	0.14	41,41,41,41	0
58	MG	1A	3689	1/1	0.92	0.28	47,47,47,47	0
58	MG	2A	3431	1/1	0.92	0.29	49,49,49,49	0
58	MG	2A	3675	1/1	0.92	0.18	46,46,46,46	0
58	MG	2a	1627	1/1	0.92	0.21	89,89,89,89	0
58	MG	2A	3432	1/1	0.92	0.21	56,56,56,56	0
58	MG	1A	3470	1/1	0.92	0.14	67,67,67,67	0
58	MG	1A	3471	1/1	0.92	0.34	59,59,59,59	0
58	MG	2A	3440	1/1	0.92	0.15	77,77,77,77	0
58	MG	2A	3442	1/1	0.92	0.33	86,86,86,86	0
58	MG	1A	3118	1/1	0.92	0.30	46,46,46,46	0
58	MG	1A	3926	1/1	0.92	0.16	37,37,37,37	0
58	MG	1P	205	1/1	0.92	0.18	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	4046	1/1	0.92	0.16	43,43,43,43	0
58	MG	1A	3179	1/1	0.92	0.54	46,46,46,46	0
58	MG	2a	1640	1/1	0.92	0.06	74,74,74,74	0
58	MG	2A	3691	1/1	0.92	0.20	53,53,53,53	0
58	MG	1A	3084	1/1	0.92	0.18	37,37,37,37	0
58	MG	1A	4050	1/1	0.92	0.23	33,33,33,33	0
58	MG	1A	3182	1/1	0.92	0.13	58,58,58,58	0
58	MG	2A	3697	1/1	0.92	0.08	71,71,71,71	0
58	MG	1A	3067	1/1	0.92	0.09	58,58,58,58	0
58	MG	1A	3304	1/1	0.92	0.45	45,45,45,45	0
58	MG	2A	3149	1/1	0.92	0.18	62,62,62,62	0
58	MG	1A	3533	1/1	0.92	0.23	44,44,44,44	0
58	MG	2A	3703	1/1	0.92	0.25	74,74,74,74	0
58	MG	1A	3075	1/1	0.92	0.17	36,36,36,36	0
58	MG	1A	3216	1/1	0.92	0.36	44,44,44,44	0
58	MG	1A	3053	1/1	0.92	0.49	62,62,62,62	0
58	MG	2A	3710	1/1	0.92	0.34	69,69,69,69	0
58	MG	1A	3943	1/1	0.92	0.15	61,61,61,61	0
58	MG	1A	3623	1/1	0.92	0.18	27,27,27,27	0
58	MG	1A	3715	1/1	0.92	0.16	72,72,72,72	0
58	MG	2A	3001	1/1	0.92	0.36	70,70,70,70	0
58	MG	2a	1669	1/1	0.92	0.10	83,83,83,83	0
58	MG	2A	3477	1/1	0.92	0.21	39,39,39,39	0
58	MG	2A	3727	1/1	0.92	0.12	78,78,78,78	0
58	MG	1V	202	1/1	0.92	0.49	48,48,48,48	0
58	MG	2A	3480	1/1	0.92	0.16	67,67,67,67	0
58	MG	1A	3716	1/1	0.92	0.20	68,68,68,68	0
58	MG	1A	3719	1/1	0.92	0.10	54,54,54,54	0
58	MG	1A	3625	1/1	0.92	0.16	54,54,54,54	0
58	MG	2A	3488	1/1	0.92	0.16	72,72,72,72	0
58	MG	2a	1684	1/1	0.92	0.30	75,75,75,75	0
58	MG	2A	3309	1/1	0.92	0.24	70,70,70,70	0
58	MG	1A	3723	1/1	0.92	0.06	68,68,68,68	0
58	MG	1X	102	1/1	0.92	0.33	48,48,48,48	0
58	MG	1Z	301	1/1	0.92	0.29	62,62,62,62	0
58	MG	2A	3012	1/1	0.92	0.12	47,47,47,47	0
58	MG	2A	3167	1/1	0.92	0.40	65,65,65,65	0
58	MG	2A	3747	1/1	0.92	0.05	59,59,59,59	0
58	MG	2A	3317	1/1	0.92	0.12	76,76,76,76	0
58	MG	1A	3843	1/1	0.92	0.13	53,53,53,53	0
58	MG	2A	3510	1/1	0.92	0.23	74,74,74,74	0
58	MG	1A	4077	1/1	0.92	0.17	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1a	1697	1/1	0.92	0.49	80,80,80,80	0
58	MG	2A	3173	1/1	0.92	0.18	65,65,65,65	0
58	MG	1a	1698	1/1	0.92	0.39	70,70,70,70	0
58	MG	10	104	1/1	0.92	0.29	52,52,52,52	0
58	MG	2A	3179	1/1	0.92	0.15	70,70,70,70	0
58	MG	1A	3218	1/1	0.92	0.14	45,45,45,45	0
58	MG	1A	4079	1/1	0.92	0.27	31,31,31,31	0
58	MG	2A	3765	1/1	0.92	0.15	69,69,69,69	0
58	MG	1a	1703	1/1	0.92	0.28	77,77,77,77	0
58	MG	1A	3015	1/1	0.92	0.21	46,46,46,46	0
58	MG	1A	3964	1/1	0.92	0.17	56,56,56,56	0
58	MG	2A	3187	1/1	0.92	0.71	73,73,73,73	0
58	MG	1A	4084	1/1	0.92	0.13	63,63,63,63	0
58	MG	2A	3773	1/1	0.92	0.33	72,72,72,72	0
58	MG	1A	4085	1/1	0.92	0.17	63,63,63,63	0
58	MG	2A	3035	1/1	0.92	0.29	71,71,71,71	0
58	MG	1A	3102	1/1	0.92	0.16	42,42,42,42	0
58	MG	2A	3782	1/1	0.92	0.12	80,80,80,80	0
58	MG	1B	201	1/1	0.92	0.19	73,73,73,73	0
58	MG	15	105	1/1	0.92	0.46	38,38,38,38	0
58	MG	1A	3850	1/1	0.92	0.07	44,44,44,44	0
58	MG	1A	3066	1/1	0.92	0.16	38,38,38,38	0
58	MG	2A	3197	1/1	0.92	0.19	63,63,63,63	0
58	MG	15	108	1/1	0.92	0.10	63,63,63,63	0
58	MG	2a	1739	1/1	0.92	0.24	61,61,61,61	0
58	MG	2A	3563	1/1	0.92	0.18	51,51,51,51	0
58	MG	16	102	1/1	0.92	0.14	64,64,64,64	0
58	MG	2A	3797	1/1	0.92	0.23	73,73,73,73	0
58	MG	1A	3491	1/1	0.92	0.21	34,34,34,34	0
58	MG	1A	3547	1/1	0.92	0.47	51,51,51,51	0
58	MG	1A	3189	1/1	0.92	0.50	50,50,50,50	0
58	MG	1A	3109	1/1	0.92	0.18	46,46,46,46	0
58	MG	2B	202	1/1	0.92	0.10	74,74,74,74	0
58	MG	1A	3642	1/1	0.92	0.13	38,38,38,38	0
58	MG	1A	3749	1/1	0.92	0.21	35,35,35,35	0
58	MG	1a	1724	1/1	0.92	0.37	61,61,61,61	0
58	MG	1a	1725	1/1	0.92	0.10	77,77,77,77	0
58	MG	1B	219	1/1	0.92	0.14	59,59,59,59	0
58	MG	1A	3194	1/1	0.92	0.53	44,44,44,44	0
58	MG	2A	3361	1/1	0.92	0.30	75,75,75,75	0
58	MG	2a	1773	1/1	0.92	0.24	77,77,77,77	0
58	MG	2a	1775	1/1	0.92	0.15	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3268	1/1	0.92	0.59	61,61,61,61	0
58	MG	2B	212	1/1	0.92	0.16	86,86,86,86	0
58	MG	1A	3985	1/1	0.92	0.11	75,75,75,75	0
58	MG	1a	1730	1/1	0.92	0.28	69,69,69,69	0
58	MG	2a	1780	1/1	0.92	0.33	73,73,73,73	0
58	MG	1a	1608	1/1	0.92	0.17	71,71,71,71	0
58	MG	1A	3083	1/1	0.92	0.19	47,47,47,47	0
58	MG	1a	1745	1/1	0.92	0.14	54,54,54,54	0
58	MG	1A	3875	1/1	0.92	0.15	37,37,37,37	0
58	MG	2a	1789	1/1	0.92	0.10	76,76,76,76	0
58	MG	1A	3399	1/1	0.92	0.11	44,44,44,44	0
58	MG	1A	3878	1/1	0.92	0.16	35,35,35,35	0
58	MG	2E	306	1/1	0.92	0.22	51,51,51,51	0
58	MG	2a	1798	1/1	0.92	0.33	72,72,72,72	0
58	MG	1A	3166	1/1	0.92	0.14	38,38,38,38	0
58	MG	1A	3112	1/1	0.92	0.18	47,47,47,47	0
58	MG	1A	3202	1/1	0.92	0.09	53,53,53,53	0
58	MG	1A	3404	1/1	0.92	0.12	60,60,60,60	0
58	MG	1a	1767	1/1	0.92	0.10	81,81,81,81	0
58	MG	2F	306	1/1	0.92	0.19	65,65,65,65	0
58	MG	1a	1770	1/1	0.92	0.15	78,78,78,78	0
58	MG	1A	3887	1/1	0.92	0.25	59,59,59,59	0
58	MG	2a	1808	1/1	0.92	0.16	73,73,73,73	0
58	MG	2N	201	1/1	0.92	0.25	73,73,73,73	0
58	MG	1A	3659	1/1	0.92	0.20	32,32,32,32	0
58	MG	1A	3661	1/1	0.92	0.12	67,67,67,67	0
58	MG	2A	3085	1/1	0.92	0.07	61,61,61,61	0
58	MG	2A	3612	1/1	0.92	0.11	75,75,75,75	0
58	MG	2T	201	1/1	0.92	0.19	72,72,72,72	0
58	MG	2A	3613	1/1	0.92	0.18	57,57,57,57	0
58	MG	2T	204	1/1	0.92	0.13	74,74,74,74	0
58	MG	1a	1624	1/1	0.92	0.11	63,63,63,63	0
58	MG	1A	3505	1/1	0.92	0.50	57,57,57,57	0
58	MG	2W	202	1/1	0.92	0.32	63,63,63,63	0
58	MG	1E	309	1/1	0.92	0.14	60,60,60,60	0
58	MG	1A	3238	1/1	0.92	0.17	43,43,43,43	0
58	MG	1A	3776	1/1	0.92	0.22	59,59,59,59	0
58	MG	2A	3624	1/1	0.92	0.29	62,62,62,62	0
58	MG	1A	3894	1/1	0.92	0.14	53,53,53,53	0
58	MG	1a	1789	1/1	0.92	0.09	85,85,85,85	0
58	MG	2A	3094	1/1	0.92	0.18	86,86,86,86	0
58	MG	1A	3276	1/1	0.92	0.18	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3396	1/1	0.92	0.17	70,70,70,70	0
58	MG	1a	1638	1/1	0.92	0.07	56,56,56,56	0
58	MG	1A	3284	1/1	0.92	0.11	56,56,56,56	0
58	MG	1A	3904	1/1	0.92	0.22	70,70,70,70	0
58	MG	1A	3905	1/1	0.92	0.12	44,44,44,44	0
58	MG	2x	105	1/1	0.92	0.41	80,80,80,80	0
58	MG	1F	308	1/1	0.92	0.17	67,67,67,67	0
58	MG	2A	3103	1/1	0.92	0.09	59,59,59,59	0
58	MG	1A	3239	1/1	0.92	0.16	43,43,43,43	0
58	MG	2A	3645	1/1	0.92	0.22	79,79,79,79	0
58	MG	1a	1803	1/1	0.92	0.20	69,69,69,69	0
61	ZN	19	102	1/1	0.92	0.36	104,104,104,104	0
61	ZN	24	501	1/1	0.92	0.20	140,140,140,140	0
58	MG	1A	3241	1/1	0.92	0.48	46,46,46,46	0
58	MG	1A	3242	1/1	0.92	0.12	55,55,55,55	0
58	MG	1A	3833	1/1	0.93	0.28	55,55,55,55	0
58	MG	2A	3490	1/1	0.93	0.22	56,56,56,56	0
58	MG	1A	3610	1/1	0.93	0.12	59,59,59,59	0
58	MG	1A	3745	1/1	0.93	0.11	52,52,52,52	0
58	MG	1A	3746	1/1	0.93	0.12	35,35,35,35	0
58	MG	1A	3425	1/1	0.93	0.25	45,45,45,45	0
58	MG	2A	3711	1/1	0.93	0.11	50,50,50,50	0
58	MG	2A	3712	1/1	0.93	0.15	78,78,78,78	0
58	MG	1a	1636	1/1	0.93	0.10	86,86,86,86	0
58	MG	1A	3329	1/1	0.93	0.24	64,64,64,64	0
58	MG	1A	3937	1/1	0.93	0.12	55,55,55,55	0
58	MG	2A	3507	1/1	0.93	0.06	75,75,75,75	0
58	MG	1a	1773	1/1	0.93	0.17	63,63,63,63	0
58	MG	1A	3017	1/1	0.93	0.37	60,60,60,60	0
58	MG	1A	3621	1/1	0.93	0.22	46,46,46,46	0
58	MG	2A	3514	1/1	0.93	0.27	60,60,60,60	0
58	MG	1A	3457	1/1	0.93	0.24	53,53,53,53	0
58	MG	1A	3277	1/1	0.93	0.20	33,33,33,33	0
58	MG	2A	3210	1/1	0.93	0.57	68,68,68,68	0
58	MG	2A	3734	1/1	0.93	0.38	87,87,87,87	0
58	MG	2A	3525	1/1	0.93	0.20	70,70,70,70	0
58	MG	1A	3687	1/1	0.93	0.18	39,39,39,39	0
58	MG	2a	1659	1/1	0.93	0.22	58,58,58,58	0
58	MG	2A	3344	1/1	0.93	0.14	66,66,66,66	0
58	MG	1O	205	1/1	0.93	0.19	82,82,82,82	0
58	MG	2A	3079	1/1	0.93	0.16	62,62,62,62	0
58	MG	1A	3945	1/1	0.93	0.12	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1a	1784	1/1	0.93	0.26	69,69,69,69	0
58	MG	2A	3534	1/1	0.93	0.30	62,62,62,62	0
58	MG	1A	3853	1/1	0.93	0.20	43,43,43,43	0
58	MG	1A	3406	1/1	0.93	0.25	47,47,47,47	0
58	MG	2A	3752	1/1	0.93	0.17	52,52,52,52	0
58	MG	2a	1673	1/1	0.93	0.15	73,73,73,73	0
58	MG	1Q	204	1/1	0.93	0.18	46,46,46,46	0
58	MG	2A	3541	1/1	0.93	0.23	46,46,46,46	0
58	MG	2A	3542	1/1	0.93	0.23	48,48,48,48	0
58	MG	1Q	205	1/1	0.93	0.18	76,76,76,76	0
58	MG	1A	3950	1/1	0.93	0.13	31,31,31,31	0
58	MG	2A	3547	1/1	0.93	0.38	52,52,52,52	0
58	MG	1Q	207	1/1	0.93	0.17	54,54,54,54	0
58	MG	1A	3951	1/1	0.93	0.11	66,66,66,66	0
58	MG	1R	201	1/1	0.93	0.19	53,53,53,53	0
58	MG	1a	1660	1/1	0.93	0.14	83,83,83,83	0
58	MG	1a	1804	1/1	0.93	0.05	91,91,91,91	0
58	MG	1A	3434	1/1	0.93	0.57	56,56,56,56	0
58	MG	1A	4061	1/1	0.93	0.18	58,58,58,58	0
58	MG	1A	3568	1/1	0.93	0.72	51,51,51,51	0
58	MG	1A	3863	1/1	0.93	0.11	69,69,69,69	0
58	MG	1A	3570	1/1	0.93	0.21	54,54,54,54	0
58	MG	1A	3959	1/1	0.93	0.11	72,72,72,72	0
58	MG	2A	3778	1/1	0.93	0.08	75,75,75,75	0
58	MG	1A	3007	1/1	0.93	0.18	39,39,39,39	0
58	MG	2A	3372	1/1	0.93	0.34	77,77,77,77	0
58	MG	1e	202	1/1	0.93	0.19	81,81,81,81	0
58	MG	1A	4072	1/1	0.93	0.10	72,72,72,72	0
58	MG	2A	3785	1/1	0.93	0.12	66,66,66,66	0
58	MG	1A	3201	1/1	0.93	0.25	38,38,38,38	0
58	MG	1a	1672	1/1	0.93	0.19	80,80,80,80	0
58	MG	1A	3694	1/1	0.93	0.20	58,58,58,58	0
58	MG	2a	1714	1/1	0.93	0.14	82,82,82,82	0
58	MG	1A	3695	1/1	0.93	0.10	87,87,87,87	0
58	MG	1A	3966	1/1	0.93	0.07	76,76,76,76	0
58	MG	2A	3113	1/1	0.93	0.40	56,56,56,56	0
58	MG	1A	3777	1/1	0.93	0.24	33,33,33,33	0
58	MG	1A	3780	1/1	0.93	0.23	26,26,26,26	0
58	MG	2a	1723	1/1	0.93	0.05	79,79,79,79	0
58	MG	1A	3972	1/1	0.93	0.27	69,69,69,69	0
58	MG	1A	3781	1/1	0.93	0.26	52,52,52,52	0
58	MG	1A	3782	1/1	0.93	0.11	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3335	1/1	0.93	0.27	67,67,67,67	0
58	MG	1a	1685	1/1	0.93	0.12	66,66,66,66	0
58	MG	1A	3883	1/1	0.93	0.14	35,35,35,35	0
58	MG	10	101	1/1	0.93	0.46	57,57,57,57	0
58	MG	2A	3392	1/1	0.93	0.35	70,70,70,70	0
58	MG	2A	3596	1/1	0.93	0.22	57,57,57,57	0
58	MG	2A	3127	1/1	0.93	0.21	60,60,60,60	0
58	MG	1A	3980	1/1	0.93	0.17	40,40,40,40	0
58	MG	2a	1740	1/1	0.93	0.19	72,72,72,72	0
58	MG	2a	1741	1/1	0.93	0.28	76,76,76,76	0
58	MG	1A	3249	1/1	0.93	0.25	78,78,78,78	0
58	MG	2a	1744	1/1	0.93	0.13	86,86,86,86	0
58	MG	2A	3604	1/1	0.93	0.05	80,80,80,80	0
58	MG	2A	3397	1/1	0.93	0.28	70,70,70,70	0
58	MG	1A	3442	1/1	0.93	0.27	53,53,53,53	0
58	MG	1A	3702	1/1	0.93	0.28	55,55,55,55	0
58	MG	1x	105	1/1	0.93	0.27	71,71,71,71	0
58	MG	1A	3639	1/1	0.93	0.26	62,62,62,62	0
58	MG	2a	1755	1/1	0.93	0.09	87,87,87,87	0
58	MG	2D	304	1/1	0.93	1.02	53,53,53,53	0
58	MG	2A	3269	1/1	0.93	0.29	74,74,74,74	0
58	MG	2E	301	1/1	0.93	0.32	77,77,77,77	0
58	MG	1A	3793	1/1	0.93	0.17	50,50,50,50	0
58	MG	2A	3615	1/1	0.93	0.24	45,45,45,45	0
58	MG	2A	3616	1/1	0.93	0.22	76,76,76,76	0
58	MG	1A	3641	1/1	0.93	0.22	43,43,43,43	0
58	MG	2A	3618	1/1	0.93	0.21	53,53,53,53	0
58	MG	2a	1766	1/1	0.93	0.12	74,74,74,74	0
58	MG	1A	3039	1/1	0.93	0.22	65,65,65,65	0
58	MG	1A	3991	1/1	0.93	0.18	52,52,52,52	0
58	MG	1y	101	1/1	0.93	0.15	70,70,70,70	0
58	MG	13	102	1/1	0.93	0.30	51,51,51,51	0
58	MG	1A	3534	1/1	0.93	0.33	60,60,60,60	0
58	MG	15	103	1/1	0.93	0.42	47,47,47,47	0
58	MG	1A	3358	1/1	0.93	0.23	52,52,52,52	0
58	MG	1A	3998	1/1	0.93	0.07	70,70,70,70	0
58	MG	1B	226	1/1	0.93	0.14	53,53,53,53	0
58	MG	2Q	201	1/1	0.93	0.12	61,61,61,61	0
58	MG	1B	227	1/1	0.93	0.11	47,47,47,47	0
58	MG	2a	1787	1/1	0.93	0.07	73,73,73,73	0
58	MG	2a	1788	1/1	0.93	0.13	75,75,75,75	0
58	MG	1A	3414	1/1	0.93	0.36	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3011	1/1	0.93	0.12	64,64,64,64	0
58	MG	2a	1794	1/1	0.93	0.23	75,75,75,75	0
58	MG	2A	3639	1/1	0.93	0.26	74,74,74,74	0
58	MG	2a	1796	1/1	0.93	0.16	89,89,89,89	0
58	MG	2A	3423	1/1	0.93	0.22	69,69,69,69	0
58	MG	17	103	1/1	0.93	0.31	40,40,40,40	0
58	MG	1A	3807	1/1	0.93	0.16	50,50,50,50	0
58	MG	2A	3429	1/1	0.93	0.30	66,66,66,66	0
58	MG	2A	3290	1/1	0.93	0.10	61,61,61,61	0
58	MG	1B	230	1/1	0.93	0.21	81,81,81,81	0
58	MG	1A	3292	1/1	0.93	0.19	48,48,48,48	0
58	MG	2A	3294	1/1	0.93	0.15	77,77,77,77	0
58	MG	1A	3271	1/1	0.93	0.19	49,49,49,49	0
58	MG	1A	3475	1/1	0.93	0.18	47,47,47,47	0
58	MG	1A	3906	1/1	0.93	0.18	83,83,83,83	0
58	MG	1A	3476	1/1	0.93	0.44	56,56,56,56	0
58	MG	1A	3722	1/1	0.93	0.09	60,60,60,60	0
58	MG	2A	3026	1/1	0.93	0.43	65,65,65,65	0
58	MG	2A	3302	1/1	0.93	0.26	79,79,79,79	0
58	MG	1A	3818	1/1	0.93	0.15	48,48,48,48	0
58	MG	1A	4014	1/1	0.93	0.08	59,59,59,59	0
58	MG	2A	3665	1/1	0.93	0.12	70,70,70,70	0
58	MG	1A	3009	1/1	0.93	0.21	35,35,35,35	0
58	MG	2A	3454	1/1	0.93	0.24	71,71,71,71	0
58	MG	1A	3724	1/1	0.93	0.25	26,26,26,26	0
58	MG	2a	1603	1/1	0.93	0.09	76,76,76,76	0
58	MG	1a	1610	1/1	0.93	0.09	82,82,82,82	0
58	MG	1A	3509	1/1	0.93	0.33	40,40,40,40	0
58	MG	2A	3177	1/1	0.93	0.22	64,64,64,64	0
58	MG	1A	3593	1/1	0.93	0.17	73,73,73,73	0
58	MG	2a	1608	1/1	0.93	0.33	89,89,89,89	0
58	MG	2A	3677	1/1	0.93	0.41	56,56,56,56	0
58	MG	2A	3463	1/1	0.93	0.21	56,56,56,56	0
58	MG	2A	3464	1/1	0.93	0.13	64,64,64,64	0
58	MG	1A	3253	1/1	0.93	0.14	40,40,40,40	0
58	MG	2v	101	1/1	0.93	0.54	85,85,85,85	0
58	MG	2A	3313	1/1	0.93	0.31	77,77,77,77	0
58	MG	1a	1616	1/1	0.93	0.18	68,68,68,68	0
58	MG	2x	102	1/1	0.93	0.32	61,61,61,61	0
58	MG	1A	4025	1/1	0.93	0.06	82,82,82,82	0
58	MG	1A	3043	1/1	0.93	0.16	46,46,46,46	0
58	MG	1A	3298	1/1	0.93	0.40	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	3424	1/1	0.93	0.40	51,51,51,51	0
58	MG	1a	1740	1/1	0.93	0.08	71,71,71,71	0
58	MG	2A	3478	1/1	0.93	0.33	69,69,69,69	0
58	MG	1a	1741	1/1	0.93	0.07	74,74,74,74	0
58	MG	1A	3920	1/1	0.93	0.10	64,64,64,64	0
60	CLM	2w	103	20/20	0.93	0.23	51,55,72,76	0
58	MG	1A	3922	1/1	0.93	0.11	78,78,78,78	0
58	MG	1A	3673	1/1	0.93	0.20	28,28,28,28	0
58	MG	1A	3741	1/1	0.93	0.29	25,25,25,25	0
58	MG	1a	1627	1/1	0.93	0.16	64,64,64,64	0
58	MG	1B	225	1/1	0.94	0.27	68,68,68,68	0
58	MG	1A	3223	1/1	0.94	0.31	63,63,63,63	0
58	MG	1A	3135	1/1	0.94	0.23	53,53,53,53	0
58	MG	2A	3247	1/1	0.94	0.22	74,74,74,74	0
58	MG	1A	3873	1/1	0.94	0.14	48,48,48,48	0
58	MG	2A	3648	1/1	0.94	0.24	67,67,67,67	0
58	MG	1A	3159	1/1	0.94	0.23	44,44,44,44	0
58	MG	1a	1752	1/1	0.94	0.13	89,89,89,89	0
58	MG	1a	1753	1/1	0.94	0.25	54,54,54,54	0
58	MG	1A	3520	1/1	0.94	0.07	91,91,91,91	0
58	MG	1A	3768	1/1	0.94	0.16	40,40,40,40	0
58	MG	1A	3770	1/1	0.94	0.09	49,49,49,49	0
58	MG	1B	233	1/1	0.94	0.19	60,60,60,60	0
58	MG	1a	1766	1/1	0.94	0.15	81,81,81,81	0
58	MG	1a	1612	1/1	0.94	0.07	78,78,78,78	0
58	MG	1a	1768	1/1	0.94	0.12	69,69,69,69	0
58	MG	1A	3880	1/1	0.94	0.17	41,41,41,41	0
58	MG	2A	3664	1/1	0.94	0.37	47,47,47,47	0
58	MG	1A	3990	1/1	0.94	0.26	59,59,59,59	0
58	MG	1A	3262	1/1	0.94	0.19	77,77,77,77	0
58	MG	2A	3439	1/1	0.94	0.17	68,68,68,68	0
58	MG	1A	3344	1/1	0.94	0.32	49,49,49,49	0
58	MG	1a	1774	1/1	0.94	0.14	66,66,66,66	0
58	MG	2A	3671	1/1	0.94	0.20	67,67,67,67	0
58	MG	1A	3678	1/1	0.94	0.11	43,43,43,43	0
58	MG	2A	3673	1/1	0.94	0.10	75,75,75,75	0
58	MG	2A	3674	1/1	0.94	0.26	76,76,76,76	0
58	MG	1A	3523	1/1	0.94	0.14	61,61,61,61	0
58	MG	1D	3610	1/1	0.94	0.30	80,80,80,80	0
58	MG	2A	3100	1/1	0.94	0.18	38,38,38,38	0
58	MG	1D	3611	1/1	0.94	0.32	45,45,45,45	0
58	MG	2A	3680	1/1	0.94	0.12	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3136	1/1	0.94	0.32	37,37,37,37	0
58	MG	1A	3525	1/1	0.94	0.45	55,55,55,55	0
58	MG	1E	306	1/1	0.94	0.18	42,42,42,42	0
58	MG	1A	3229	1/1	0.94	0.64	46,46,46,46	0
58	MG	1a	1786	1/1	0.94	0.16	79,79,79,79	0
58	MG	2A	3280	1/1	0.94	0.29	60,60,60,60	0
58	MG	1A	3348	1/1	0.94	0.21	43,43,43,43	0
58	MG	2a	1649	1/1	0.94	0.14	81,81,81,81	0
58	MG	1A	3115	1/1	0.94	0.54	50,50,50,50	0
58	MG	2A	3690	1/1	0.94	0.20	65,65,65,65	0
58	MG	1A	3594	1/1	0.94	0.11	41,41,41,41	0
58	MG	2A	3692	1/1	0.94	0.28	48,48,48,48	0
58	MG	1A	3199	1/1	0.94	0.22	29,29,29,29	0
58	MG	1E	314	1/1	0.94	0.28	61,61,61,61	0
58	MG	1a	1634	1/1	0.94	0.24	40,40,40,40	0
58	MG	2A	3467	1/1	0.94	0.24	48,48,48,48	0
58	MG	2A	3287	1/1	0.94	0.21	63,63,63,63	0
58	MG	1a	1800	1/1	0.94	0.15	66,66,66,66	0
58	MG	1A	4008	1/1	0.94	0.17	51,51,51,51	0
58	MG	2A	3120	1/1	0.94	0.24	73,73,73,73	0
58	MG	1A	3437	1/1	0.94	0.40	62,62,62,62	0
58	MG	2A	3704	1/1	0.94	0.06	86,86,86,86	0
58	MG	2A	3705	1/1	0.94	0.10	70,70,70,70	0
58	MG	1A	4012	1/1	0.94	0.20	51,51,51,51	0
58	MG	1A	3598	1/1	0.94	0.20	42,42,42,42	0
58	MG	1A	3601	1/1	0.94	0.23	40,40,40,40	0
58	MG	2a	1674	1/1	0.94	0.27	63,63,63,63	0
58	MG	2A	3126	1/1	0.94	0.17	59,59,59,59	0
58	MG	1A	4015	1/1	0.94	0.12	72,72,72,72	0
58	MG	1F	310	1/1	0.94	0.17	65,65,65,65	0
58	MG	2A	3129	1/1	0.94	0.22	62,62,62,62	0
58	MG	2A	3486	1/1	0.94	0.12	62,62,62,62	0
58	MG	2a	1683	1/1	0.94	0.23	67,67,67,67	0
58	MG	1a	1643	1/1	0.94	0.21	65,65,65,65	0
58	MG	2A	3720	1/1	0.94	0.10	70,70,70,70	0
58	MG	1a	1812	1/1	0.94	0.20	68,68,68,68	0
58	MG	2A	3722	1/1	0.94	0.05	83,83,83,83	0
58	MG	2a	1689	1/1	0.94	0.21	85,85,85,85	0
58	MG	1a	1813	1/1	0.94	0.09	69,69,69,69	0
58	MG	1a	1814	1/1	0.94	0.20	64,64,64,64	0
58	MG	2a	1693	1/1	0.94	0.12	80,80,80,80	0
58	MG	1A	3902	1/1	0.94	0.36	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	1G	201	1/1	0.94	0.13	51,51,51,51	0
58	MG	1A	3603	1/1	0.94	0.26	39,39,39,39	0
58	MG	1A	3139	1/1	0.94	0.29	50,50,50,50	0
58	MG	1A	3440	1/1	0.94	0.24	45,45,45,45	0
58	MG	2A	3501	1/1	0.94	0.18	80,80,80,80	0
58	MG	2A	3502	1/1	0.94	0.25	55,55,55,55	0
58	MG	1A	3141	1/1	0.94	0.20	25,25,25,25	0
58	MG	2A	3505	1/1	0.94	0.27	67,67,67,67	0
58	MG	2a	1707	1/1	0.94	0.26	86,86,86,86	0
58	MG	1a	1651	1/1	0.94	0.23	71,71,71,71	0
58	MG	1A	3315	1/1	0.94	0.35	68,68,68,68	0
58	MG	2A	3146	1/1	0.94	0.22	66,66,66,66	0
58	MG	1A	3802	1/1	0.94	0.15	49,49,49,49	0
58	MG	1A	3805	1/1	0.94	0.10	39,39,39,39	0
58	MG	1A	3168	1/1	0.94	0.26	70,70,70,70	0
58	MG	1A	3203	1/1	0.94	0.20	32,32,32,32	0
58	MG	1A	3617	1/1	0.94	0.19	39,39,39,39	0
58	MG	2A	3521	1/1	0.94	0.21	75,75,75,75	0
58	MG	2A	3523	1/1	0.94	0.20	63,63,63,63	0
58	MG	2A	3524	1/1	0.94	0.19	70,70,70,70	0
58	MG	1A	3812	1/1	0.94	0.30	58,58,58,58	0
58	MG	1O	204	1/1	0.94	0.16	68,68,68,68	0
58	MG	1A	3813	1/1	0.94	0.30	71,71,71,71	0
58	MG	2A	3529	1/1	0.94	0.16	72,72,72,72	0
58	MG	1A	3619	1/1	0.94	0.11	72,72,72,72	0
58	MG	1A	3021	1/1	0.94	0.21	34,34,34,34	0
58	MG	1A	3119	1/1	0.94	0.17	47,47,47,47	0
58	MG	1A	3543	1/1	0.94	0.38	63,63,63,63	0
58	MG	2a	1734	1/1	0.94	0.16	79,79,79,79	0
58	MG	1A	3105	1/1	0.94	0.17	34,34,34,34	0
58	MG	1A	3713	1/1	0.94	0.19	29,29,29,29	0
58	MG	2A	3537	1/1	0.94	0.17	48,48,48,48	0
58	MG	1A	3243	1/1	0.94	0.14	55,55,55,55	0
58	MG	1A	3822	1/1	0.94	0.26	53,53,53,53	0
58	MG	2A	3775	1/1	0.94	0.05	86,86,86,86	0
58	MG	2A	3776	1/1	0.94	0.14	85,85,85,85	0
58	MG	1A	3932	1/1	0.94	0.23	34,34,34,34	0
58	MG	2a	1743	1/1	0.94	0.11	78,78,78,78	0
58	MG	1A	3546	1/1	0.94	0.47	70,70,70,70	0
58	MG	1A	3717	1/1	0.94	0.13	67,67,67,67	0
58	MG	1a	1677	1/1	0.94	0.14	77,77,77,77	0
58	MG	2a	1749	1/1	0.94	0.08	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3207	1/1	0.94	0.22	63,63,63,63	0
58	MG	1A	3548	1/1	0.94	0.23	43,43,43,43	0
58	MG	1A	3106	1/1	0.94	0.49	50,50,50,50	0
58	MG	2A	3554	1/1	0.94	0.34	53,53,53,53	0
58	MG	2A	3555	1/1	0.94	0.21	58,58,58,58	0
58	MG	2A	3557	1/1	0.94	0.14	51,51,51,51	0
58	MG	2A	3558	1/1	0.94	0.23	65,65,65,65	0
58	MG	2A	3176	1/1	0.94	0.14	52,52,52,52	0
58	MG	1A	3550	1/1	0.94	0.23	41,41,41,41	0
58	MG	2A	3795	1/1	0.94	0.17	53,53,53,53	0
58	MG	1A	3287	1/1	0.94	0.17	56,56,56,56	0
58	MG	2a	1763	1/1	0.94	0.20	73,73,73,73	0
58	MG	1A	3407	1/1	0.94	0.28	72,72,72,72	0
58	MG	1A	3209	1/1	0.94	0.22	44,44,44,44	0
58	MG	1A	3730	1/1	0.94	0.25	55,55,55,55	0
58	MG	1A	3840	1/1	0.94	0.15	42,42,42,42	0
58	MG	1A	3947	1/1	0.94	0.16	43,43,43,43	0
58	MG	1A	4065	1/1	0.94	0.09	63,63,63,63	0
58	MG	2A	3571	1/1	0.94	0.35	68,68,68,68	0
58	MG	1A	3147	1/1	0.94	0.17	39,39,39,39	0
58	MG	1A	3027	1/1	0.94	0.05	79,79,79,79	0
58	MG	1A	3291	1/1	0.94	0.34	37,37,37,37	0
58	MG	1A	4071	1/1	0.94	0.19	29,29,29,29	0
58	MG	1X	105	1/1	0.94	0.20	60,60,60,60	0
58	MG	1Y	201	1/1	0.94	0.10	71,71,71,71	0
58	MG	2A	3019	1/1	0.94	0.17	46,46,46,46	0
58	MG	1A	3149	1/1	0.94	0.16	33,33,33,33	0
58	MG	1Z	302	1/1	0.94	0.06	75,75,75,75	0
58	MG	1a	1700	1/1	0.94	0.24	62,62,62,62	0
58	MG	2a	1791	1/1	0.94	0.29	69,69,69,69	0
58	MG	2B	217	1/1	0.94	0.21	80,80,80,80	0
58	MG	1A	3123	1/1	0.94	0.36	45,45,45,45	0
58	MG	2A	3027	1/1	0.94	0.08	45,45,45,45	0
58	MG	2D	302	1/1	0.94	0.28	59,59,59,59	0
58	MG	2A	3200	1/1	0.94	0.39	70,70,70,70	0
58	MG	1A	3091	1/1	0.94	0.15	63,63,63,63	0
58	MG	2A	3031	1/1	0.94	0.18	69,69,69,69	0
58	MG	1A	3849	1/1	0.94	0.14	51,51,51,51	0
58	MG	1A	3955	1/1	0.94	0.12	51,51,51,51	0
58	MG	1A	3059	1/1	0.94	0.16	40,40,40,40	0
58	MG	1A	3957	1/1	0.94	0.21	64,64,64,64	0
58	MG	10	107	1/1	0.94	0.23	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3153	1/1	0.94	0.11	32,32,32,32	0
58	MG	2A	3597	1/1	0.94	0.21	74,74,74,74	0
58	MG	2A	3598	1/1	0.94	0.24	82,82,82,82	0
58	MG	11	102	1/1	0.94	0.20	54,54,54,54	0
58	MG	2A	3600	1/1	0.94	0.10	88,88,88,88	0
58	MG	2A	3378	1/1	0.94	0.58	75,75,75,75	0
58	MG	2A	3039	1/1	0.94	0.27	42,42,42,42	0
58	MG	2A	3603	1/1	0.94	0.20	76,76,76,76	0
58	MG	1A	3960	1/1	0.94	0.18	73,73,73,73	0
58	MG	2a	1816	1/1	0.94	0.20	87,87,87,87	0
58	MG	1A	4083	1/1	0.94	0.23	82,82,82,82	0
58	MG	1A	3961	1/1	0.94	0.16	76,76,76,76	0
58	MG	1A	3852	1/1	0.94	0.27	47,47,47,47	0
58	MG	2R	201	1/1	0.94	0.18	58,58,58,58	0
58	MG	2A	3610	1/1	0.94	0.10	70,70,70,70	0
58	MG	1A	3130	1/1	0.94	0.12	68,68,68,68	0
58	MG	1a	1716	1/1	0.94	0.34	80,80,80,80	0
58	MG	2A	3048	1/1	0.94	0.21	63,63,63,63	0
58	MG	1A	3854	1/1	0.94	0.09	46,46,46,46	0
58	MG	2j	201	1/1	0.94	0.07	84,84,84,84	0
58	MG	2V	201	1/1	0.94	0.11	70,70,70,70	0
58	MG	2A	3221	1/1	0.94	0.49	61,61,61,61	0
58	MG	1A	3855	1/1	0.94	0.29	40,40,40,40	0
58	MG	1A	3466	1/1	0.94	0.17	60,60,60,60	0
58	MG	1A	3063	1/1	0.94	0.19	45,45,45,45	0
58	MG	1A	3660	1/1	0.94	0.14	34,34,34,34	0
58	MG	2w	101	1/1	0.94	0.12	98,98,98,98	0
58	MG	1A	3575	1/1	0.94	0.27	52,52,52,52	0
58	MG	1A	3864	1/1	0.94	0.16	36,36,36,36	0
58	MG	21	101	1/1	0.94	0.17	80,80,80,80	0
58	MG	23	101	1/1	0.94	0.15	72,72,72,72	0
58	MG	23	102	1/1	0.94	0.27	75,75,75,75	0
58	MG	16	103	1/1	0.94	0.30	64,64,64,64	0
58	MG	17	101	1/1	0.94	0.23	41,41,41,41	0
58	MG	1A	3663	1/1	0.94	0.23	32,32,32,32	0
58	MG	1A	3258	1/1	0.94	0.16	41,41,41,41	0
58	MG	1B	216	1/1	0.94	0.09	61,61,61,61	0
58	MG	1A	3977	1/1	0.94	0.25	43,43,43,43	0
58	MG	19	101	1/1	0.94	0.21	58,58,58,58	0
61	ZN	14	501	1/1	0.94	0.08	115,115,115,115	0
58	MG	1a	1736	1/1	0.94	0.16	60,60,60,60	0
58	MG	1a	1738	1/1	0.94	0.32	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3666	1/1	0.94	0.16	45,45,45,45	0
58	MG	1A	3979	1/1	0.94	0.20	31,31,31,31	0
58	MG	1A	3835	1/1	0.95	0.21	47,47,47,47	0
58	MG	1W	205	1/1	0.95	0.33	50,50,50,50	0
58	MG	1W	207	1/1	0.95	0.18	32,32,32,32	0
58	MG	1a	1780	1/1	0.95	0.12	84,84,84,84	0
58	MG	2A	3714	1/1	0.95	0.17	80,80,80,80	0
58	MG	2A	3527	1/1	0.95	0.28	54,54,54,54	0
58	MG	2A	3717	1/1	0.95	0.18	69,69,69,69	0
58	MG	2a	1645	1/1	0.95	0.11	80,80,80,80	0
58	MG	1X	101	1/1	0.95	0.80	50,50,50,50	0
58	MG	2A	3348	1/1	0.95	0.47	72,72,72,72	0
58	MG	1A	3474	1/1	0.95	0.14	55,55,55,55	0
58	MG	1B	221	1/1	0.95	0.15	74,74,74,74	0
58	MG	1a	1785	1/1	0.95	0.16	75,75,75,75	0
58	MG	2a	1651	1/1	0.95	0.92	80,80,80,80	0
58	MG	2A	3725	1/1	0.95	0.17	65,65,65,65	0
58	MG	1A	4009	1/1	0.95	0.13	49,49,49,49	0
58	MG	1A	4010	1/1	0.95	0.21	45,45,45,45	0
58	MG	2a	1655	1/1	0.95	0.12	91,91,91,91	0
58	MG	2A	3074	1/1	0.95	0.30	52,52,52,52	0
58	MG	2A	3358	1/1	0.95	0.27	71,71,71,71	0
58	MG	1a	1790	1/1	0.95	0.20	77,77,77,77	0
58	MG	2A	3539	1/1	0.95	0.10	63,63,63,63	0
58	MG	1A	3755	1/1	0.95	0.20	27,27,27,27	0
58	MG	2a	1662	1/1	0.95	0.12	70,70,70,70	0
58	MG	2A	3736	1/1	0.95	0.09	82,82,82,82	0
58	MG	1A	3252	1/1	0.95	0.33	53,53,53,53	0
58	MG	1a	1669	1/1	0.95	0.10	77,77,77,77	0
58	MG	2a	1667	1/1	0.95	0.09	56,56,56,56	0
58	MG	2A	3543	1/1	0.95	0.13	83,83,83,83	0
58	MG	1A	3375	1/1	0.95	0.41	64,64,64,64	0
58	MG	2A	3742	1/1	0.95	0.17	66,66,66,66	0
58	MG	1A	3351	1/1	0.95	0.22	49,49,49,49	0
58	MG	1A	3196	1/1	0.95	0.08	56,56,56,56	0
58	MG	1A	3931	1/1	0.95	0.07	52,52,52,52	0
58	MG	1A	3628	1/1	0.95	0.18	42,42,42,42	0
58	MG	1A	3764	1/1	0.95	0.32	70,70,70,70	0
58	MG	2a	1676	1/1	0.95	0.22	75,75,75,75	0
58	MG	2A	3225	1/1	0.95	0.33	58,58,58,58	0
58	MG	1A	3765	1/1	0.95	0.23	32,32,32,32	0
58	MG	1A	3326	1/1	0.95	0.32	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	1678	1/1	0.95	0.16	65,65,65,65	0
58	MG	2A	3090	1/1	0.95	0.63	56,56,56,56	0
58	MG	1B	237	1/1	0.95	0.23	46,46,46,46	0
58	MG	2A	3231	1/1	0.95	0.32	69,69,69,69	0
58	MG	1a	1810	1/1	0.95	0.20	80,80,80,80	0
58	MG	1A	3197	1/1	0.95	0.22	43,43,43,43	0
58	MG	2A	3565	1/1	0.95	0.13	64,64,64,64	0
58	MG	2A	3762	1/1	0.95	0.19	52,52,52,52	0
58	MG	1a	1681	1/1	0.95	0.12	81,81,81,81	0
58	MG	2A	3567	1/1	0.95	0.25	57,57,57,57	0
58	MG	1A	4026	1/1	0.95	0.16	59,59,59,59	0
58	MG	2A	3381	1/1	0.95	0.27	68,68,68,68	0
58	MG	2A	3096	1/1	0.95	0.12	68,68,68,68	0
58	MG	2a	1698	1/1	0.95	0.18	90,90,90,90	0
58	MG	1A	3769	1/1	0.95	0.21	54,54,54,54	0
58	MG	2A	3573	1/1	0.95	0.19	82,82,82,82	0
58	MG	2A	3772	1/1	0.95	0.25	60,60,60,60	0
58	MG	1A	3116	1/1	0.95	0.38	39,39,39,39	0
58	MG	1A	3140	1/1	0.95	0.26	46,46,46,46	0
58	MG	13	104	1/1	0.95	0.21	58,58,58,58	0
58	MG	1A	4032	1/1	0.95	0.16	55,55,55,55	0
58	MG	15	104	1/1	0.95	0.20	39,39,39,39	0
58	MG	1A	3633	1/1	0.95	0.10	62,62,62,62	0
58	MG	2A	3246	1/1	0.95	0.28	61,61,61,61	0
58	MG	1A	3634	1/1	0.95	0.17	50,50,50,50	0
58	MG	2A	3783	1/1	0.95	0.18	40,40,40,40	0
58	MG	2A	3107	1/1	0.95	0.27	72,72,72,72	0
58	MG	1k	201	1/1	0.95	0.23	56,56,56,56	0
58	MG	1A	3383	1/1	0.95	0.25	35,35,35,35	0
58	MG	1A	3701	1/1	0.95	0.34	56,56,56,56	0
58	MG	2A	3252	1/1	0.95	0.08	89,89,89,89	0
58	MG	16	101	1/1	0.95	0.40	57,57,57,57	0
58	MG	2a	1721	1/1	0.95	0.14	81,81,81,81	0
58	MG	1A	3485	1/1	0.95	0.23	47,47,47,47	0
58	MG	2A	3793	1/1	0.95	0.31	47,47,47,47	0
58	MG	2A	3590	1/1	0.95	0.10	56,56,56,56	0
58	MG	1p	101	1/1	0.95	0.11	77,77,77,77	0
58	MG	1A	3384	1/1	0.95	0.34	71,71,71,71	0
58	MG	1t	201	1/1	0.95	0.08	63,63,63,63	0
58	MG	2a	1730	1/1	0.95	0.15	79,79,79,79	0
58	MG	1A	3529	1/1	0.95	0.28	61,61,61,61	0
58	MG	17	102	1/1	0.95	0.15	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	3034	1/1	0.95	0.18	42,42,42,42	0
58	MG	2A	3262	1/1	0.95	0.40	89,89,89,89	0
58	MG	2A	3409	1/1	0.95	0.33	56,56,56,56	0
58	MG	2A	3263	1/1	0.95	0.20	76,76,76,76	0
58	MG	1E	313	1/1	0.95	0.33	46,46,46,46	0
58	MG	1A	3279	1/1	0.95	0.17	40,40,40,40	0
58	MG	18	104	1/1	0.95	0.18	53,53,53,53	0
58	MG	1A	4043	1/1	0.95	0.29	41,41,41,41	0
58	MG	2B	208	1/1	0.95	0.13	93,93,93,93	0
58	MG	1A	3417	1/1	0.95	0.10	67,67,67,67	0
58	MG	1w	109	1/1	0.95	0.15	80,80,80,80	0
58	MG	2a	1745	1/1	0.95	0.14	76,76,76,76	0
58	MG	1A	3868	1/1	0.95	0.20	29,29,29,29	0
58	MG	1A	3787	1/1	0.95	0.19	25,25,25,25	0
58	MG	2B	213	1/1	0.95	0.21	74,74,74,74	0
58	MG	2a	1750	1/1	0.95	0.29	62,62,62,62	0
58	MG	1A	3709	1/1	0.95	0.11	54,54,54,54	0
58	MG	1A	3281	1/1	0.95	0.43	42,42,42,42	0
58	MG	2A	3426	1/1	0.95	0.14	67,67,67,67	0
58	MG	1A	3388	1/1	0.95	0.20	47,47,47,47	0
58	MG	1A	3282	1/1	0.95	0.40	55,55,55,55	0
58	MG	1A	3876	1/1	0.95	0.21	31,31,31,31	0
58	MG	2A	3278	1/1	0.95	0.25	75,75,75,75	0
58	MG	2a	1758	1/1	0.95	0.08	93,93,93,93	0
58	MG	1A	3795	1/1	0.95	0.07	66,66,66,66	0
58	MG	1x	111	1/1	0.95	0.29	66,66,66,66	0
58	MG	2A	3434	1/1	0.95	0.12	75,75,75,75	0
58	MG	1G	203	1/1	0.95	0.10	59,59,59,59	0
58	MG	1A	3536	1/1	0.95	0.52	55,55,55,55	0
58	MG	1A	3035	1/1	0.95	0.17	55,55,55,55	0
58	MG	1A	3167	1/1	0.95	0.21	39,39,39,39	0
58	MG	1a	1718	1/1	0.95	0.25	80,80,80,80	0
58	MG	2a	1767	1/1	0.95	0.17	69,69,69,69	0
58	MG	1A	3074	1/1	0.95	0.09	39,39,39,39	0
58	MG	2a	1774	1/1	0.95	0.29	76,76,76,76	0
58	MG	2A	3634	1/1	0.95	0.18	44,44,44,44	0
58	MG	2A	3147	1/1	0.95	0.06	90,90,90,90	0
58	MG	1A	3801	1/1	0.95	0.09	58,58,58,58	0
58	MG	1A	3967	1/1	0.95	0.11	58,58,58,58	0
58	MG	1A	3132	1/1	0.95	0.13	45,45,45,45	0
58	MG	2A	3450	1/1	0.95	0.35	70,70,70,70	0
58	MG	1A	3970	1/1	0.95	0.12	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3452	1/1	0.95	0.16	46,46,46,46	0
58	MG	1A	3426	1/1	0.95	0.16	57,57,57,57	0
58	MG	1A	3427	1/1	0.95	0.13	55,55,55,55	0
58	MG	2A	3013	1/1	0.95	0.19	58,58,58,58	0
58	MG	1A	3662	1/1	0.95	0.16	60,60,60,60	0
58	MG	1A	3428	1/1	0.95	0.17	56,56,56,56	0
58	MG	2a	1790	1/1	0.95	0.32	73,73,73,73	0
58	MG	1A	3811	1/1	0.95	0.22	61,61,61,61	0
58	MG	2T	203	1/1	0.95	0.18	60,60,60,60	0
58	MG	2a	1793	1/1	0.95	0.14	70,70,70,70	0
58	MG	1A	3222	1/1	0.95	0.19	40,40,40,40	0
58	MG	2A	3300	1/1	0.95	0.36	64,64,64,64	0
58	MG	1A	3731	1/1	0.95	0.15	46,46,46,46	0
58	MG	1a	1732	1/1	0.95	0.25	63,63,63,63	0
58	MG	1A	3113	1/1	0.95	0.09	51,51,51,51	0
58	MG	1A	3895	1/1	0.95	0.32	72,72,72,72	0
58	MG	2Y	201	1/1	0.95	0.22	63,63,63,63	0
58	MG	1A	3896	1/1	0.95	0.20	40,40,40,40	0
58	MG	2A	3472	1/1	0.95	0.08	76,76,76,76	0
58	MG	1A	3897	1/1	0.95	0.25	40,40,40,40	0
58	MG	1A	3054	1/1	0.95	0.17	41,41,41,41	0
58	MG	1A	3176	1/1	0.95	0.26	38,38,38,38	0
58	MG	1a	1743	1/1	0.95	0.21	64,64,64,64	0
58	MG	2a	1807	1/1	0.95	0.23	61,61,61,61	0
58	MG	1a	1744	1/1	0.95	0.21	63,63,63,63	0
58	MG	2a	1809	1/1	0.95	0.07	80,80,80,80	0
58	MG	2A	3172	1/1	0.95	0.20	72,72,72,72	0
58	MG	2A	3668	1/1	0.95	0.08	62,62,62,62	0
58	MG	1a	1635	1/1	0.95	0.25	84,84,84,84	0
58	MG	2A	3174	1/1	0.95	0.27	71,71,71,71	0
58	MG	1A	3433	1/1	0.95	0.25	73,73,73,73	0
58	MG	2A	3482	1/1	0.95	0.25	67,67,67,67	0
58	MG	1A	3177	1/1	0.95	0.21	26,26,26,26	0
58	MG	2a	1817	1/1	0.95	0.13	91,91,91,91	0
58	MG	1R	206	1/1	0.95	0.23	40,40,40,40	0
58	MG	2a	1819	1/1	0.95	0.29	60,60,60,60	0
58	MG	1A	3227	1/1	0.95	0.23	48,48,48,48	0
58	MG	2A	3487	1/1	0.95	0.20	42,42,42,42	0
58	MG	1A	3743	1/1	0.95	0.17	54,54,54,54	0
58	MG	1a	1755	1/1	0.95	0.24	75,75,75,75	0
58	MG	2A	3679	1/1	0.95	0.15	69,69,69,69	0
58	MG	1A	3613	1/1	0.95	0.16	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3491	1/1	0.95	0.13	77,77,77,77	0
58	MG	2A	3041	1/1	0.95	0.26	64,64,64,64	0
58	MG	2A	3493	1/1	0.95	0.25	63,63,63,63	0
58	MG	2A	3494	1/1	0.95	0.24	50,50,50,50	0
58	MG	1a	1758	1/1	0.95	0.13	75,75,75,75	0
58	MG	1A	3677	1/1	0.95	0.22	52,52,52,52	0
58	MG	1A	3513	1/1	0.95	0.58	45,45,45,45	0
58	MG	1B	204	1/1	0.95	0.23	70,70,70,70	0
58	MG	1A	3556	1/1	0.95	0.08	75,75,75,75	0
58	MG	1A	3228	1/1	0.95	0.31	40,40,40,40	0
58	MG	2A	3050	1/1	0.95	0.17	37,37,37,37	0
58	MG	2a	1618	1/1	0.95	0.14	91,91,91,91	0
58	MG	1a	1647	1/1	0.95	0.34	74,74,74,74	0
58	MG	1a	1769	1/1	0.95	0.10	80,80,80,80	0
58	MG	2A	3695	1/1	0.95	0.12	73,73,73,73	0
58	MG	1U	207	1/1	0.95	0.68	44,44,44,44	0
58	MG	2A	3509	1/1	0.95	0.17	59,59,59,59	0
58	MG	1A	3750	1/1	0.95	0.22	50,50,50,50	0
58	MG	2A	3511	1/1	0.95	0.22	39,39,39,39	0
58	MG	2A	3196	1/1	0.95	0.11	68,68,68,68	0
58	MG	1A	3065	1/1	0.95	0.29	36,36,36,36	0
58	MG	1A	3752	1/1	0.95	0.18	40,40,40,40	0
58	MG	1V	205	1/1	0.95	0.30	59,59,59,59	0
58	MG	2A	3340	1/1	0.95	0.17	66,66,66,66	0
61	ZN	1n	103	1/1	0.95	0.11	87,87,87,87	0
58	MG	1A	3620	1/1	0.95	0.10	57,57,57,57	0
61	ZN	26	102	1/1	0.95	0.14	74,74,74,74	0
58	MG	1A	3834	1/1	0.95	0.27	28,28,28,28	0
58	MG	2A	3522	1/1	0.95	0.26	67,67,67,67	0
58	MG	1A	3086	1/1	0.96	0.46	55,55,55,55	0
58	MG	2A	3744	1/1	0.96	0.13	58,58,58,58	0
58	MG	1A	3595	1/1	0.96	0.22	57,57,57,57	0
58	MG	1A	3720	1/1	0.96	0.08	63,63,63,63	0
58	MG	2A	3104	1/1	0.96	0.17	62,62,62,62	0
58	MG	2a	1663	1/1	0.96	0.07	68,68,68,68	0
58	MG	2A	3105	1/1	0.96	0.14	52,52,52,52	0
58	MG	2A	3394	1/1	0.96	0.42	69,69,69,69	0
58	MG	2A	3751	1/1	0.96	0.32	49,49,49,49	0
58	MG	1A	3655	1/1	0.96	0.23	33,33,33,33	0
58	MG	1A	3311	1/1	0.96	0.16	66,66,66,66	0
58	MG	2A	3108	1/1	0.96	0.15	62,62,62,62	0
58	MG	1A	3100	1/1	0.96	0.10	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	1A	3117	1/1	0.96	0.27	42,42,42,42	0
58	MG	2A	3757	1/1	0.96	0.26	69,69,69,69	0
58	MG	1A	3599	1/1	0.96	0.16	18,18,18,18	0
58	MG	18	101	1/1	0.96	0.25	52,52,52,52	0
58	MG	1A	3728	1/1	0.96	0.11	75,75,75,75	0
58	MG	1A	3013	1/1	0.96	0.23	35,35,35,35	0
58	MG	2a	1677	1/1	0.96	0.14	76,76,76,76	0
58	MG	2A	3258	1/1	0.96	0.28	64,64,64,64	0
58	MG	1A	3602	1/1	0.96	0.10	73,73,73,73	0
58	MG	2A	3116	1/1	0.96	0.20	48,48,48,48	0
58	MG	2A	3583	1/1	0.96	0.11	73,73,73,73	0
58	MG	1A	3804	1/1	0.96	0.08	38,38,38,38	0
58	MG	2A	3410	1/1	0.96	0.29	55,55,55,55	0
58	MG	1A	3881	1/1	0.96	0.14	47,47,47,47	0
58	MG	2a	1686	1/1	0.96	0.05	77,77,77,77	0
58	MG	1A	3014	1/1	0.96	0.16	33,33,33,33	0
58	MG	1A	3732	1/1	0.96	0.20	44,44,44,44	0
58	MG	1A	3552	1/1	0.96	0.23	43,43,43,43	0
58	MG	1A	4055	1/1	0.96	0.27	67,67,67,67	0
58	MG	2A	3591	1/1	0.96	0.13	71,71,71,71	0
58	MG	2a	1692	1/1	0.96	0.29	67,67,67,67	0
58	MG	2A	3123	1/1	0.96	0.15	81,81,81,81	0
58	MG	1A	3607	1/1	0.96	0.15	59,59,59,59	0
58	MG	1A	3735	1/1	0.96	0.16	46,46,46,46	0
58	MG	2A	3270	1/1	0.96	0.20	68,68,68,68	0
58	MG	1A	3076	1/1	0.96	0.33	58,58,58,58	0
58	MG	1x	104	1/1	0.96	0.19	84,84,84,84	0
58	MG	2a	1700	1/1	0.96	0.14	73,73,73,73	0
58	MG	1A	3285	1/1	0.96	0.16	58,58,58,58	0
58	MG	1A	3889	1/1	0.96	0.32	36,36,36,36	0
58	MG	1A	3814	1/1	0.96	0.17	64,64,64,64	0
58	MG	2a	1704	1/1	0.96	0.09	84,84,84,84	0
58	MG	1A	4063	1/1	0.96	0.15	36,36,36,36	0
58	MG	1A	3030	1/1	0.96	0.41	36,36,36,36	0
58	MG	2A	3789	1/1	0.96	0.20	40,40,40,40	0
58	MG	1x	110	1/1	0.96	0.09	69,69,69,69	0
58	MG	2A	3791	1/1	0.96	0.22	57,57,57,57	0
58	MG	1A	3482	1/1	0.96	0.08	61,61,61,61	0
58	MG	1A	3742	1/1	0.96	0.20	53,53,53,53	0
58	MG	2A	3606	1/1	0.96	0.30	65,65,65,65	0
58	MG	1A	3676	1/1	0.96	0.25	34,34,34,34	0
58	MG	2A	3436	1/1	0.96	0.24	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	1715	1/1	0.96	0.17	72,72,72,72	0
58	MG	1A	3008	1/1	0.96	0.19	31,31,31,31	0
58	MG	1A	3211	1/1	0.96	0.41	42,42,42,42	0
58	MG	2A	3799	1/1	0.96	0.24	74,74,74,74	0
58	MG	1A	3616	1/1	0.96	0.12	70,70,70,70	0
58	MG	2A	3441	1/1	0.96	0.29	60,60,60,60	0
58	MG	1P	201	1/1	0.96	0.57	40,40,40,40	0
58	MG	1P	202	1/1	0.96	0.48	46,46,46,46	0
58	MG	2A	3145	1/1	0.96	0.22	70,70,70,70	0
58	MG	2A	3446	1/1	0.96	0.24	69,69,69,69	0
58	MG	1P	204	1/1	0.96	0.39	41,41,41,41	0
58	MG	1a	1731	1/1	0.96	0.22	81,81,81,81	0
58	MG	2A	3621	1/1	0.96	0.27	71,71,71,71	0
58	MG	2A	3148	1/1	0.96	0.24	79,79,79,79	0
58	MG	1A	3561	1/1	0.96	0.18	43,43,43,43	0
58	MG	1a	1734	1/1	0.96	0.23	56,56,56,56	0
58	MG	1a	1625	1/1	0.96	0.26	67,67,67,67	0
58	MG	2A	3152	1/1	0.96	0.26	61,61,61,61	0
58	MG	2A	3627	1/1	0.96	0.19	75,75,75,75	0
58	MG	2A	3628	1/1	0.96	0.24	74,74,74,74	0
58	MG	1a	1626	1/1	0.96	0.11	79,79,79,79	0
58	MG	1a	1737	1/1	0.96	0.19	35,35,35,35	0
58	MG	2A	3632	1/1	0.96	0.25	42,42,42,42	0
58	MG	2A	3633	1/1	0.96	0.22	44,44,44,44	0
58	MG	2A	3456	1/1	0.96	0.37	64,64,64,64	0
58	MG	2A	3457	1/1	0.96	0.20	58,58,58,58	0
58	MG	1A	3235	1/1	0.96	0.40	37,37,37,37	0
58	MG	1a	1739	1/1	0.96	0.19	49,49,49,49	0
58	MG	1Q	203	1/1	0.96	0.22	37,37,37,37	0
58	MG	2A	3461	1/1	0.96	0.19	59,59,59,59	0
58	MG	2A	3640	1/1	0.96	0.16	53,53,53,53	0
58	MG	2E	305	1/1	0.96	0.22	68,68,68,68	0
58	MG	1A	3683	1/1	0.96	0.22	36,36,36,36	0
58	MG	1A	3563	1/1	0.96	0.28	43,43,43,43	0
58	MG	1A	3827	1/1	0.96	0.09	63,63,63,63	0
58	MG	2A	3022	1/1	0.96	0.36	58,58,58,58	0
58	MG	1a	1632	1/1	0.96	0.43	68,68,68,68	0
58	MG	2A	3646	1/1	0.96	0.20	44,44,44,44	0
58	MG	1A	3236	1/1	0.96	0.24	39,39,39,39	0
58	MG	1a	1746	1/1	0.96	0.30	51,51,51,51	0
58	MG	1A	3107	1/1	0.96	0.73	43,43,43,43	0
58	MG	2A	3028	1/1	0.96	0.28	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	3029	1/1	0.96	0.29	87,87,87,87	0
58	MG	2A	3311	1/1	0.96	0.12	60,60,60,60	0
58	MG	1a	1748	1/1	0.96	0.18	81,81,81,81	0
58	MG	1a	1749	1/1	0.96	0.28	70,70,70,70	0
58	MG	2A	3656	1/1	0.96	0.20	73,73,73,73	0
58	MG	1A	3108	1/1	0.96	0.36	39,39,39,39	0
58	MG	2a	1768	1/1	0.96	0.30	76,76,76,76	0
58	MG	2a	1772	1/1	0.96	0.12	81,81,81,81	0
58	MG	1A	3909	1/1	0.96	0.14	69,69,69,69	0
58	MG	1R	204	1/1	0.96	0.32	49,49,49,49	0
58	MG	1A	3567	1/1	0.96	0.23	39,39,39,39	0
58	MG	1A	3294	1/1	0.96	0.39	75,75,75,75	0
58	MG	1a	1756	1/1	0.96	0.06	75,75,75,75	0
58	MG	1A	3993	1/1	0.96	0.14	43,43,43,43	0
58	MG	1A	3627	1/1	0.96	0.23	24,24,24,24	0
58	MG	1A	3527	1/1	0.96	0.41	59,59,59,59	0
58	MG	2a	1781	1/1	0.96	0.12	82,82,82,82	0
58	MG	1a	1762	1/1	0.96	0.22	71,71,71,71	0
58	MG	2A	3181	1/1	0.96	0.18	76,76,76,76	0
58	MG	2A	3326	1/1	0.96	0.15	48,48,48,48	0
58	MG	1T	201	1/1	0.96	0.12	77,77,77,77	0
58	MG	1A	3571	1/1	0.96	0.26	46,46,46,46	0
58	MG	2A	3044	1/1	0.96	0.15	76,76,76,76	0
58	MG	1U	202	1/1	0.96	0.35	47,47,47,47	0
58	MG	1A	3169	1/1	0.96	0.11	43,43,43,43	0
58	MG	1B	206	1/1	0.96	0.29	55,55,55,55	0
58	MG	1A	3839	1/1	0.96	0.20	32,32,32,32	0
58	MG	2A	3049	1/1	0.96	0.22	62,62,62,62	0
58	MG	25	103	1/1	0.96	0.48	61,61,61,61	0
58	MG	1B	208	1/1	0.96	0.18	55,55,55,55	0
58	MG	1A	4002	1/1	0.96	0.20	40,40,40,40	0
58	MG	1A	3763	1/1	0.96	0.14	59,59,59,59	0
58	MG	1A	3240	1/1	0.96	0.81	39,39,39,39	0
58	MG	1A	3919	1/1	0.96	0.19	52,52,52,52	0
58	MG	2A	3056	1/1	0.96	0.33	75,75,75,75	0
58	MG	1A	3265	1/1	0.96	0.25	46,46,46,46	0
58	MG	1B	215	1/1	0.96	0.15	61,61,61,61	0
58	MG	1A	3049	1/1	0.96	0.29	34,34,34,34	0
58	MG	1a	1658	1/1	0.96	0.24	76,76,76,76	0
58	MG	1B	218	1/1	0.96	0.21	47,47,47,47	0
58	MG	1A	3699	1/1	0.96	0.16	43,43,43,43	0
58	MG	2A	3515	1/1	0.96	0.13	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	3925	1/1	0.96	0.17	42,42,42,42	0
58	MG	1A	3001	1/1	0.96	0.16	43,43,43,43	0
58	MG	2A	3205	1/1	0.96	0.28	61,61,61,61	0
58	MG	2A	3520	1/1	0.96	0.17	72,72,72,72	0
58	MG	1B	222	1/1	0.96	0.24	60,60,60,60	0
58	MG	2A	3066	1/1	0.96	0.45	73,73,73,73	0
58	MG	1X	104	1/1	0.96	0.47	53,53,53,53	0
58	MG	1A	3010	1/1	0.96	0.13	39,39,39,39	0
58	MG	1A	3497	1/1	0.96	0.21	77,77,77,77	0
58	MG	2A	3357	1/1	0.96	0.33	54,54,54,54	0
58	MG	1A	3772	1/1	0.96	0.19	30,30,30,30	0
58	MG	1A	3173	1/1	0.96	0.42	46,46,46,46	0
58	MG	1A	3302	1/1	0.96	0.29	59,59,59,59	0
58	MG	1A	3334	1/1	0.96	0.26	62,62,62,62	0
58	MG	2A	3075	1/1	0.96	0.23	54,54,54,54	0
58	MG	1a	1794	1/1	0.96	0.17	68,68,68,68	0
58	MG	2A	3077	1/1	0.96	0.22	40,40,40,40	0
58	MG	1a	1795	1/1	0.96	0.28	64,64,64,64	0
58	MG	2a	1626	1/1	0.96	0.24	98,98,98,98	0
58	MG	10	102	1/1	0.96	0.23	56,56,56,56	0
58	MG	1A	3538	1/1	0.96	0.27	57,57,57,57	0
58	MG	1A	3175	1/1	0.96	0.14	44,44,44,44	0
58	MG	1A	4022	1/1	0.96	0.12	60,60,60,60	0
58	MG	1A	3857	1/1	0.96	0.33	43,43,43,43	0
58	MG	1A	4024	1/1	0.96	0.21	68,68,68,68	0
58	MG	1A	3858	1/1	0.96	0.36	46,46,46,46	0
58	MG	1A	3095	1/1	0.96	0.32	51,51,51,51	0
58	MG	2a	1636	1/1	0.96	0.18	70,70,70,70	0
58	MG	1A	3710	1/1	0.96	0.16	57,57,57,57	0
58	MG	2A	3724	1/1	0.96	0.47	69,69,69,69	0
58	MG	1A	3942	1/1	0.96	0.19	62,62,62,62	0
58	MG	2A	3726	1/1	0.96	0.21	56,56,56,56	0
58	MG	1D	3605	1/1	0.96	0.27	41,41,41,41	0
58	MG	2A	3728	1/1	0.96	0.35	61,61,61,61	0
58	MG	2A	3550	1/1	0.96	0.14	60,60,60,60	0
58	MG	1A	3133	1/1	0.96	0.20	49,49,49,49	0
58	MG	1A	4030	1/1	0.96	0.14	47,47,47,47	0
58	MG	1A	4031	1/1	0.96	0.15	33,33,33,33	0
58	MG	1A	3248	1/1	0.96	0.42	46,46,46,46	0
60	CLM	1A	4087	20/20	0.96	0.22	29,38,62,63	0
58	MG	1b	301	1/1	0.96	0.20	90,90,90,90	0
58	MG	2A	3735	1/1	0.96	0.23	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	15	101	1/1	0.96	0.44	44,44,44,44	0
58	MG	1E	301	1/1	0.96	0.51	41,41,41,41	0
61	ZN	2Y	202	1/1	0.96	0.14	97,97,97,97	0
58	MG	1A	3011	1/1	0.96	0.12	54,54,54,54	0
58	MG	1A	3946	1/1	0.96	0.13	60,60,60,60	0
58	MG	1A	3508	1/1	0.96	0.24	37,37,37,37	0
58	MG	1E	307	1/1	0.96	0.19	44,44,44,44	0
58	MG	2A	3504	1/1	0.97	0.28	59,59,59,59	0
58	MG	1A	3193	1/1	0.97	0.54	42,42,42,42	0
58	MG	1A	3215	1/1	0.97	0.36	51,51,51,51	0
58	MG	2a	1694	1/1	0.97	0.17	65,65,65,65	0
58	MG	2A	3508	1/1	0.97	0.22	73,73,73,73	0
58	MG	2A	3657	1/1	0.97	0.14	70,70,70,70	0
58	MG	1A	4069	1/1	0.97	0.23	38,38,38,38	0
58	MG	2A	3659	1/1	0.97	0.15	51,51,51,51	0
58	MG	1A	3378	1/1	0.97	0.24	55,55,55,55	0
58	MG	1A	3047	1/1	0.97	0.14	27,27,27,27	0
58	MG	2B	215	1/1	0.97	0.27	79,79,79,79	0
58	MG	1A	3081	1/1	0.97	0.34	44,44,44,44	0
58	MG	1A	3350	1/1	0.97	0.55	40,40,40,40	0
58	MG	1O	203	1/1	0.97	0.19	56,56,56,56	0
58	MG	1A	3748	1/1	0.97	0.16	34,34,34,34	0
58	MG	1A	3903	1/1	0.97	0.49	50,50,50,50	0
58	MG	2D	303	1/1	0.97	0.29	42,42,42,42	0
58	MG	1a	1614	1/1	0.97	0.14	75,75,75,75	0
58	MG	1A	4076	1/1	0.97	0.18	58,58,58,58	0
58	MG	1A	3137	1/1	0.97	0.45	41,41,41,41	0
58	MG	1A	3416	1/1	0.97	0.09	53,53,53,53	0
58	MG	1P	203	1/1	0.97	0.17	33,33,33,33	0
58	MG	1A	3986	1/1	0.97	0.34	55,55,55,55	0
58	MG	1A	3219	1/1	0.97	0.22	51,51,51,51	0
58	MG	1A	3490	1/1	0.97	0.51	62,62,62,62	0
58	MG	1a	1733	1/1	0.97	0.20	71,71,71,71	0
58	MG	1Q	202	1/1	0.97	0.39	47,47,47,47	0
58	MG	2F	301	1/1	0.97	0.38	51,51,51,51	0
58	MG	1A	4082	1/1	0.97	0.07	48,48,48,48	0
58	MG	1A	3174	1/1	0.97	0.20	39,39,39,39	0
58	MG	1A	3454	1/1	0.97	0.37	53,53,53,53	0
58	MG	1A	3154	1/1	0.97	0.28	48,48,48,48	0
58	MG	2a	1724	1/1	0.97	0.21	77,77,77,77	0
58	MG	1A	3756	1/1	0.97	0.19	33,33,33,33	0
58	MG	2F	308	1/1	0.97	0.38	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	3133	1/1	0.97	0.67	57,57,57,57	0
58	MG	1A	3032	1/1	0.97	0.22	33,33,33,33	0
58	MG	2a	1729	1/1	0.97	0.19	90,90,90,90	0
58	MG	2A	3135	1/1	0.97	0.35	54,54,54,54	0
58	MG	2A	3536	1/1	0.97	0.17	45,45,45,45	0
58	MG	2a	1732	1/1	0.97	0.09	90,90,90,90	0
58	MG	1A	3996	1/1	0.97	0.20	31,31,31,31	0
58	MG	1A	3156	1/1	0.97	0.41	46,46,46,46	0
58	MG	1A	3178	1/1	0.97	0.14	45,45,45,45	0
58	MG	1A	3272	1/1	0.97	0.31	41,41,41,41	0
58	MG	1A	3761	1/1	0.97	0.19	27,27,27,27	0
58	MG	1A	3012	1/1	0.97	0.09	37,37,37,37	0
58	MG	1A	3697	1/1	0.97	0.17	26,26,26,26	0
58	MG	1S	202	1/1	0.97	0.25	61,61,61,61	0
58	MG	2A	3545	1/1	0.97	0.13	54,54,54,54	0
58	MG	2A	3021	1/1	0.97	0.23	39,39,39,39	0
58	MG	1B	210	1/1	0.97	0.25	56,56,56,56	0
58	MG	2A	3549	1/1	0.97	0.22	42,42,42,42	0
58	MG	2A	3404	1/1	0.97	0.26	25,25,25,25	0
58	MG	1A	3050	1/1	0.97	0.34	38,38,38,38	0
58	MG	2a	1747	1/1	0.97	0.17	83,83,83,83	0
58	MG	1A	3303	1/1	0.97	0.22	42,42,42,42	0
58	MG	2A	3025	1/1	0.97	0.24	70,70,70,70	0
58	MG	1U	201	1/1	0.97	0.19	35,35,35,35	0
58	MG	2A	3556	1/1	0.97	0.25	63,63,63,63	0
58	MG	1A	3921	1/1	0.97	0.21	18,18,18,18	0
58	MG	1A	4007	1/1	0.97	0.14	41,41,41,41	0
58	MG	1A	3637	1/1	0.97	0.14	67,67,67,67	0
58	MG	1A	3923	1/1	0.97	0.13	66,66,66,66	0
58	MG	1A	3585	1/1	0.97	0.19	30,30,30,30	0
58	MG	1A	3464	1/1	0.97	0.26	42,42,42,42	0
58	MG	1U	208	1/1	0.97	0.25	42,42,42,42	0
58	MG	1A	3640	1/1	0.97	0.19	51,51,51,51	0
58	MG	1V	201	1/1	0.97	0.39	38,38,38,38	0
58	MG	1A	3848	1/1	0.97	0.27	31,31,31,31	0
58	MG	1A	3928	1/1	0.97	0.11	44,44,44,44	0
58	MG	2A	3719	1/1	0.97	0.28	59,59,59,59	0
58	MG	1B	223	1/1	0.97	0.09	67,67,67,67	0
58	MG	1A	3929	1/1	0.97	0.11	66,66,66,66	0
58	MG	2A	3424	1/1	0.97	0.25	64,64,64,64	0
58	MG	2A	3425	1/1	0.97	0.16	65,65,65,65	0
58	MG	1A	3503	1/1	0.97	0.15	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2a	1769	1/1	0.97	0.44	66,66,66,66	0
58	MG	2a	1770	1/1	0.97	0.35	65,65,65,65	0
58	MG	2A	3292	1/1	0.97	0.19	64,64,64,64	0
58	MG	1A	3588	1/1	0.97	0.23	33,33,33,33	0
58	MG	1A	3590	1/1	0.97	0.21	29,29,29,29	0
58	MG	1W	206	1/1	0.97	0.30	53,53,53,53	0
58	MG	1a	1659	1/1	0.97	0.28	78,78,78,78	0
58	MG	2A	3169	1/1	0.97	0.30	41,41,41,41	0
58	MG	2A	3433	1/1	0.97	0.23	32,32,32,32	0
58	MG	1A	3774	1/1	0.97	0.23	59,59,59,59	0
58	MG	1A	3644	1/1	0.97	0.21	30,30,30,30	0
58	MG	1A	3096	1/1	0.97	0.11	45,45,45,45	0
58	MG	1X	103	1/1	0.97	0.39	54,54,54,54	0
58	MG	2a	1616	1/1	0.97	0.16	89,89,89,89	0
58	MG	1A	3124	1/1	0.97	0.45	40,40,40,40	0
58	MG	1A	3041	1/1	0.97	0.40	44,44,44,44	0
58	MG	1A	3712	1/1	0.97	0.13	58,58,58,58	0
58	MG	1a	1667	1/1	0.97	0.17	65,65,65,65	0
58	MG	2A	3740	1/1	0.97	0.30	61,61,61,61	0
58	MG	1a	1783	1/1	0.97	0.16	74,74,74,74	0
58	MG	1Y	203	1/1	0.97	0.24	58,58,58,58	0
58	MG	2A	3445	1/1	0.97	0.27	49,49,49,49	0
58	MG	1A	3278	1/1	0.97	0.19	46,46,46,46	0
58	MG	1A	3940	1/1	0.97	0.09	68,68,68,68	0
58	MG	1a	1787	1/1	0.97	0.19	67,67,67,67	0
58	MG	1a	1788	1/1	0.97	0.25	67,67,67,67	0
58	MG	1B	236	1/1	0.97	0.14	51,51,51,51	0
58	MG	1A	3031	1/1	0.97	0.37	42,42,42,42	0
58	MG	1A	3036	1/1	0.97	0.13	25,25,25,25	0
58	MG	1D	3602	1/1	0.97	0.16	49,49,49,49	0
58	MG	1A	3510	1/1	0.97	0.80	54,54,54,54	0
58	MG	1A	3786	1/1	0.97	0.14	25,25,25,25	0
58	MG	1A	3718	1/1	0.97	0.13	61,61,61,61	0
58	MG	1A	3788	1/1	0.97	0.13	49,49,49,49	0
58	MG	1a	1798	1/1	0.97	0.30	60,60,60,60	0
58	MG	1A	3789	1/1	0.97	0.18	32,32,32,32	0
58	MG	2A	3070	1/1	0.97	0.16	68,68,68,68	0
58	MG	1A	3790	1/1	0.97	0.35	33,33,33,33	0
58	MG	1A	3400	1/1	0.97	0.35	42,42,42,42	0
58	MG	2a	1643	1/1	0.97	0.09	80,80,80,80	0
58	MG	1A	3656	1/1	0.97	0.12	29,29,29,29	0
58	MG	1A	3872	1/1	0.97	0.17	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3764	1/1	0.97	0.21	60,60,60,60	0
58	MG	1E	305	1/1	0.97	0.12	34,34,34,34	0
58	MG	2A	3766	1/1	0.97	0.18	57,57,57,57	0
58	MG	1A	3657	1/1	0.97	0.20	24,24,24,24	0
58	MG	1A	3551	1/1	0.97	0.30	42,42,42,42	0
58	MG	1A	3600	1/1	0.97	0.20	41,41,41,41	0
58	MG	2A	3469	1/1	0.97	0.22	39,39,39,39	0
58	MG	2A	3470	1/1	0.97	0.21	44,44,44,44	0
58	MG	2A	3471	1/1	0.97	0.26	56,56,56,56	0
58	MG	1a	1809	1/1	0.97	0.23	58,58,58,58	0
58	MG	2a	1823	1/1	0.97	0.29	73,73,73,73	0
58	MG	2A	3774	1/1	0.97	0.18	38,38,38,38	0
58	MG	1A	3045	1/1	0.97	0.12	50,50,50,50	0
58	MG	2e	201	1/1	0.97	0.07	83,83,83,83	0
58	MG	15	102	1/1	0.97	0.27	38,38,38,38	0
58	MG	1a	1690	1/1	0.97	0.49	64,64,64,64	0
58	MG	1A	3725	1/1	0.97	0.12	41,41,41,41	0
58	MG	2a	1661	1/1	0.97	0.08	68,68,68,68	0
58	MG	1A	3339	1/1	0.97	0.13	64,64,64,64	0
58	MG	1A	3879	1/1	0.97	0.06	77,77,77,77	0
58	MG	2A	3781	1/1	0.97	0.12	66,66,66,66	0
58	MG	1A	3554	1/1	0.97	0.47	48,48,48,48	0
58	MG	2r	101	1/1	0.97	0.15	89,89,89,89	0
58	MG	1A	4049	1/1	0.97	0.22	57,57,57,57	0
58	MG	2A	3213	1/1	0.97	0.17	91,91,91,91	0
58	MG	1A	3370	1/1	0.97	0.39	47,47,47,47	0
58	MG	2A	3631	1/1	0.97	0.12	58,58,58,58	0
58	MG	1A	3606	1/1	0.97	0.11	50,50,50,50	0
58	MG	1F	304	1/1	0.97	0.10	50,50,50,50	0
58	MG	1A	3283	1/1	0.97	0.14	51,51,51,51	0
58	MG	1F	306	1/1	0.97	0.16	36,36,36,36	0
58	MG	1A	3669	1/1	0.97	0.15	41,41,41,41	0
58	MG	1l	201	1/1	0.97	0.10	76,76,76,76	0
58	MG	1A	3806	1/1	0.97	0.21	54,54,54,54	0
58	MG	17	104	1/1	0.97	0.40	45,45,45,45	0
58	MG	1A	3670	1/1	0.97	0.19	30,30,30,30	0
58	MG	1A	3439	1/1	0.97	0.35	59,59,59,59	0
58	MG	1a	1706	1/1	0.97	0.22	66,66,66,66	0
58	MG	2A	3495	1/1	0.97	0.14	47,47,47,47	0
58	MG	1A	3077	1/1	0.97	0.23	46,46,46,46	0
58	MG	1A	3969	1/1	0.97	0.24	69,69,69,69	0
58	MG	18	105	1/1	0.97	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	3037	1/1	0.97	0.31	46,46,46,46	0
58	MG	1A	3738	1/1	0.97	0.24	61,61,61,61	0
58	MG	1A	3612	1/1	0.97	0.13	39,39,39,39	0
58	MG	1A	3134	1/1	0.97	0.15	48,48,48,48	0
58	MG	1A	3192	1/1	0.97	0.36	40,40,40,40	0
58	MG	1A	3898	1/1	0.98	0.19	36,36,36,36	0
58	MG	1A	3899	1/1	0.98	0.14	31,31,31,31	0
58	MG	1A	3498	1/1	0.98	0.14	73,73,73,73	0
58	MG	1A	3800	1/1	0.98	0.42	37,37,37,37	0
58	MG	1E	304	1/1	0.98	0.20	41,41,41,41	0
58	MG	1A	3681	1/1	0.98	0.27	38,38,38,38	0
58	MG	2A	3607	1/1	0.98	0.17	67,67,67,67	0
58	MG	1a	1754	1/1	0.98	0.23	64,64,64,64	0
58	MG	1A	3125	1/1	0.98	0.35	31,31,31,31	0
58	MG	1A	3803	1/1	0.98	0.14	34,34,34,34	0
58	MG	1A	3126	1/1	0.98	0.39	52,52,52,52	0
58	MG	2A	3237	1/1	0.98	0.08	80,80,80,80	0
58	MG	2A	3325	1/1	0.98	0.12	68,68,68,68	0
58	MG	1A	3127	1/1	0.98	0.37	41,41,41,41	0
58	MG	2A	3419	1/1	0.98	0.16	76,76,76,76	0
58	MG	1a	1759	1/1	0.98	0.18	69,69,69,69	0
58	MG	2A	3421	1/1	0.98	0.24	73,73,73,73	0
58	MG	2A	3518	1/1	0.98	0.14	75,75,75,75	0
58	MG	2A	3240	1/1	0.98	0.12	73,73,73,73	0
58	MG	2A	3620	1/1	0.98	0.18	70,70,70,70	0
58	MG	1a	1760	1/1	0.98	0.26	61,61,61,61	0
58	MG	2a	1771	1/1	0.98	0.18	80,80,80,80	0
58	MG	1U	209	1/1	0.98	0.38	41,41,41,41	0
58	MG	1A	3023	1/1	0.98	0.21	25,25,25,25	0
58	MG	2F	302	1/1	0.98	0.10	68,68,68,68	0
58	MG	1a	1763	1/1	0.98	0.25	62,62,62,62	0
58	MG	1A	3648	1/1	0.98	0.20	41,41,41,41	0
58	MG	1A	3808	1/1	0.98	0.10	42,42,42,42	0
58	MG	1A	4019	1/1	0.98	0.12	62,62,62,62	0
58	MG	1A	4020	1/1	0.98	0.15	70,70,70,70	0
58	MG	1A	3078	1/1	0.98	0.16	31,31,31,31	0
58	MG	1W	201	1/1	0.98	0.22	48,48,48,48	0
58	MG	1F	301	1/1	0.98	0.49	50,50,50,50	0
58	MG	1F	302	1/1	0.98	0.27	42,42,42,42	0
58	MG	1W	204	1/1	0.98	0.43	50,50,50,50	0
58	MG	1A	3042	1/1	0.98	0.28	39,39,39,39	0
58	MG	2a	1786	1/1	0.98	0.35	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3437	1/1	0.98	0.07	69,69,69,69	0
58	MG	1A	3727	1/1	0.98	0.13	24,24,24,24	0
58	MG	1A	3110	1/1	0.98	0.20	41,41,41,41	0
58	MG	2a	1680	1/1	0.98	0.28	65,65,65,65	0
58	MG	1A	3862	1/1	0.98	0.17	39,39,39,39	0
58	MG	2A	3004	1/1	0.98	0.73	63,63,63,63	0
58	MG	1A	3190	1/1	0.98	0.42	48,48,48,48	0
58	MG	1A	3056	1/1	0.98	0.14	41,41,41,41	0
58	MG	1A	3589	1/1	0.98	0.17	45,45,45,45	0
58	MG	2A	3350	1/1	0.98	0.26	48,48,48,48	0
58	MG	2A	3750	1/1	0.98	0.16	58,58,58,58	0
58	MG	1A	3280	1/1	0.98	0.41	43,43,43,43	0
58	MG	2A	3009	1/1	0.98	0.20	45,45,45,45	0
58	MG	1X	106	1/1	0.98	0.17	34,34,34,34	0
58	MG	1A	3658	1/1	0.98	0.19	30,30,30,30	0
58	MG	1A	3458	1/1	0.98	0.19	55,55,55,55	0
58	MG	2A	3649	1/1	0.98	0.19	44,44,44,44	0
58	MG	2A	3548	1/1	0.98	0.11	71,71,71,71	0
58	MG	2A	3356	1/1	0.98	0.44	59,59,59,59	0
58	MG	1A	3869	1/1	0.98	0.18	38,38,38,38	0
58	MG	1A	3975	1/1	0.98	0.18	30,30,30,30	0
58	MG	2A	3552	1/1	0.98	0.20	46,46,46,46	0
58	MG	1A	3052	1/1	0.98	0.19	59,59,59,59	0
58	MG	1A	3736	1/1	0.98	0.17	29,29,29,29	0
58	MG	1A	3146	1/1	0.98	0.36	41,41,41,41	0
58	MG	1A	3778	1/1	0.98	0.21	24,24,24,24	0
58	MG	2A	3186	1/1	0.98	0.13	65,65,65,65	0
58	MG	1A	3779	1/1	0.98	0.23	32,32,32,32	0
58	MG	1A	3160	1/1	0.98	0.25	38,38,38,38	0
58	MG	1B	217	1/1	0.98	0.24	51,51,51,51	0
58	MG	1A	3825	1/1	0.98	0.16	41,41,41,41	0
58	MG	1A	3161	1/1	0.98	0.21	40,40,40,40	0
58	MG	11	101	1/1	0.98	0.69	45,45,45,45	0
58	MG	1A	3391	1/1	0.98	0.16	34,34,34,34	0
58	MG	2A	3371	1/1	0.98	0.27	59,59,59,59	0
58	MG	1a	1797	1/1	0.98	0.33	62,62,62,62	0
58	MG	1A	3665	1/1	0.98	0.23	25,25,25,25	0
58	MG	1A	3347	1/1	0.98	0.49	44,44,44,44	0
58	MG	2A	3569	1/1	0.98	0.17	68,68,68,68	0
58	MG	1A	3987	1/1	0.98	0.08	64,64,64,64	0
58	MG	1A	3704	1/1	0.98	0.22	24,24,24,24	0
58	MG	13	101	1/1	0.98	0.20	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	1719	1/1	0.98	0.11	73,73,73,73	0
58	MG	1A	3831	1/1	0.98	0.10	56,56,56,56	0
58	MG	1A	3569	1/1	0.98	0.15	44,44,44,44	0
58	MG	1A	3162	1/1	0.98	0.44	35,35,35,35	0
58	MG	1a	1806	1/1	0.98	0.23	73,73,73,73	0
58	MG	1A	3286	1/1	0.98	0.49	57,57,57,57	0
58	MG	1A	3104	1/1	0.98	0.23	36,36,36,36	0
58	MG	1A	4053	1/1	0.98	0.24	28,28,28,28	0
58	MG	1A	3994	1/1	0.98	0.15	18,18,18,18	0
58	MG	1A	3308	1/1	0.98	0.16	42,42,42,42	0
58	MG	1A	4056	1/1	0.98	0.17	42,42,42,42	0
58	MG	2A	3685	1/1	0.98	0.19	79,79,79,79	0
58	MG	2A	3483	1/1	0.98	0.22	47,47,47,47	0
58	MG	1A	3038	1/1	0.98	0.51	39,39,39,39	0
58	MG	1A	3997	1/1	0.98	0.11	40,40,40,40	0
58	MG	1A	3838	1/1	0.98	0.20	29,29,29,29	0
58	MG	1A	3604	1/1	0.98	0.15	44,44,44,44	0
58	MG	1A	3421	1/1	0.98	0.20	62,62,62,62	0
58	MG	1R	202	1/1	0.98	0.14	63,63,63,63	0
58	MG	2a	1630	1/1	0.98	0.36	66,66,66,66	0
58	MG	1A	3233	1/1	0.98	0.49	53,53,53,53	0
58	MG	1D	3603	1/1	0.98	0.25	30,30,30,30	0
58	MG	1A	3714	1/1	0.98	0.17	26,26,26,26	0
58	MG	1A	3577	1/1	0.98	0.53	49,49,49,49	0
61	ZN	15	109	1/1	0.98	0.15	56,56,56,56	0
58	MG	1A	3844	1/1	0.98	0.09	48,48,48,48	0
58	MG	2A	3053	1/1	0.98	0.05	88,88,88,88	0
58	MG	18	102	1/1	0.98	0.21	50,50,50,50	0
58	MG	1D	3607	1/1	0.98	0.15	52,52,52,52	0
58	MG	2A	3139	1/1	0.98	0.23	54,54,54,54	0
58	MG	1A	3069	1/1	0.98	0.18	25,25,25,25	0
58	MG	1A	3609	1/1	0.98	0.18	30,30,30,30	0
58	MG	1A	3856	1/1	0.99	0.23	42,42,42,42	0
58	MG	1A	3618	1/1	0.99	0.10	29,29,29,29	0
58	MG	2A	3706	1/1	0.99	0.09	62,62,62,62	0
58	MG	1A	3072	1/1	0.99	0.18	18,18,18,18	0
58	MG	1A	3022	1/1	0.99	0.17	47,47,47,47	0
58	MG	1a	1653	1/1	0.99	0.20	66,66,66,66	0
58	MG	1A	3033	1/1	0.99	0.36	37,37,37,37	0
58	MG	1A	3003	1/1	0.99	0.20	33,33,33,33	0
58	MG	1A	3685	1/1	0.99	0.17	18,18,18,18	0
58	MG	1A	3028	1/1	0.99	0.47	42,42,42,42	0

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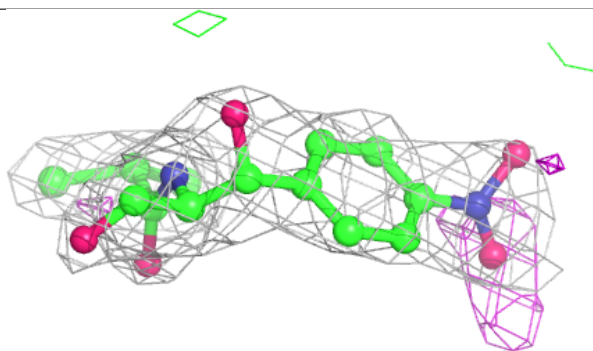
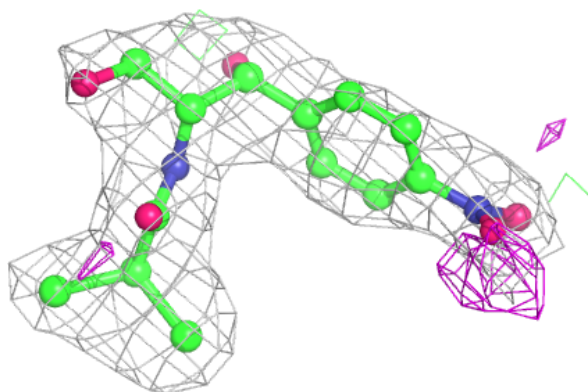
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	4068	1/1	0.99	0.24	18,18,18,18	0
58	MG	2A	3715	1/1	0.99	0.10	74,74,74,74	0
58	MG	1A	4034	1/1	0.99	0.09	61,61,61,61	0
58	MG	1A	3651	1/1	0.99	0.20	28,28,28,28	0
58	MG	1A	3624	1/1	0.99	0.25	20,20,20,20	0
58	MG	1A	3767	1/1	0.99	0.19	45,45,45,45	0
58	MG	1B	205	1/1	0.99	0.19	53,53,53,53	0
58	MG	1A	3181	1/1	0.99	0.30	56,56,56,56	0
61	ZN	1Y	204	1/1	0.99	0.15	69,69,69,69	0
58	MG	1A	3958	1/1	0.99	0.10	61,61,61,61	0
58	MG	1Y	202	1/1	0.99	0.44	60,60,60,60	0
61	ZN	16	104	1/1	0.99	0.20	50,50,50,50	0
58	MG	1D	3609	1/1	0.99	0.18	33,33,33,33	0
58	MG	2A	3506	1/1	0.99	0.20	52,52,52,52	0
58	MG	2A	3699	1/1	0.99	0.28	53,53,53,53	0
58	MG	1A	3654	1/1	0.99	0.18	46,46,46,46	0
61	ZN	25	105	1/1	0.99	0.15	84,84,84,84	0
58	MG	1A	3097	1/1	0.99	0.20	25,25,25,25	0
58	MG	1A	3667	1/1	0.99	0.20	35,35,35,35	0
58	MG	1V	204	1/1	0.99	0.34	39,39,39,39	0
62	SF4	1d	302	8/8	0.99	0.17	72,80,88,90	0
62	SF4	2d	303	8/8	0.99	0.16	74,78,87,89	0

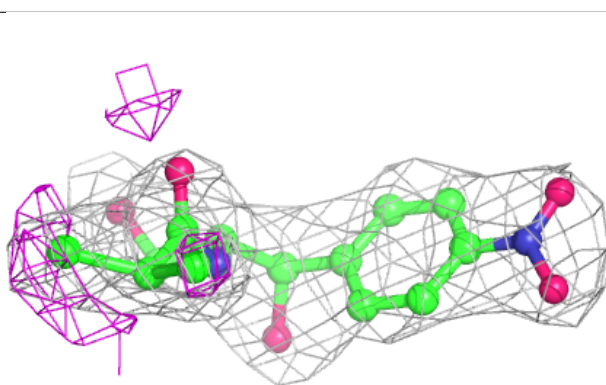
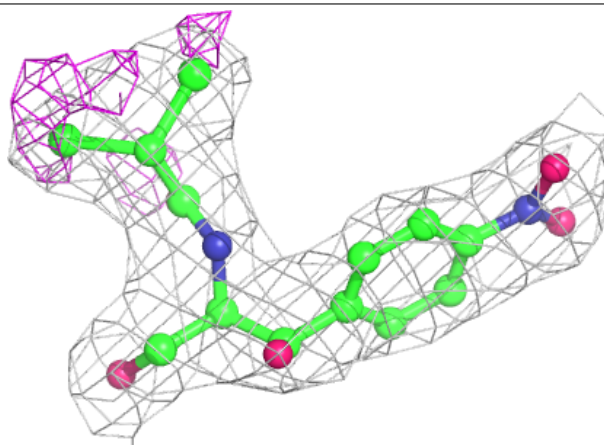
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around CLM 2w 103:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around CLM 1A 4087:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.