



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 13, 2020 – 03:31 PM EDT

PDB ID : 6CZR  
Title : The structure of amicitin bound to the 70S ribosome  
Authors : Eiler, D.R.; Steitz, T.A.; Looper, R.E.; Serrano, C.M.; Kannareddy, H.R.; Koch, M.R.; Barrows, L.R.; Testa, C.A.; Sebahar, P.R.  
Deposited on : 2018-04-09  
Resolution : 3.14 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
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)	:	2.14.6

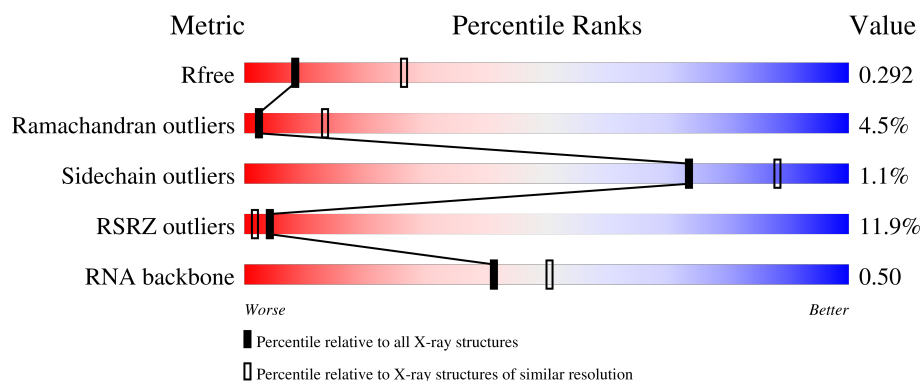
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.14 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	1626 (3.18-3.10)
Ramachandran outliers	138981	1677 (3.18-3.10)
Sidechain outliers	138945	1677 (3.18-3.10)
RSRZ outliers	127900	1588 (3.18-3.10)
RNA backbone	3102	1000 (3.46-2.82)

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

Mol	Chain	Length	Quality of chain
1	1A	2915	<div> <div>6%</div> <div>81%17%</div> </div>
1	2A	2915	<div> <div>8%</div> <div>80%19%</div> </div>
2	1B	120	<div> <div>%</div> <div>89%11%</div> </div>
2	2B	120	<div> <div>8%</div> <div>86%14%</div> </div>
3	1D	275	<div> <div></div> <div>95%5%</div> </div>

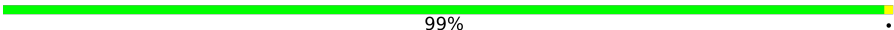

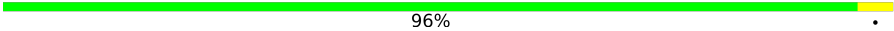

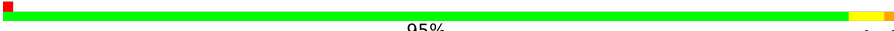

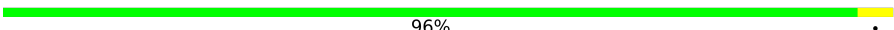

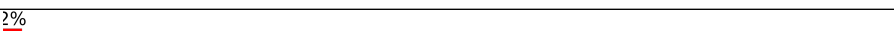
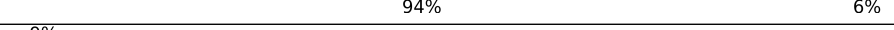
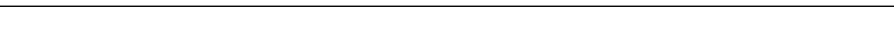
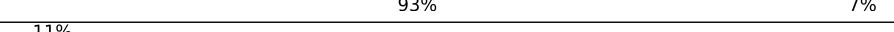


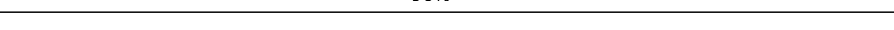
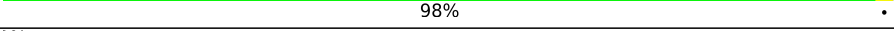
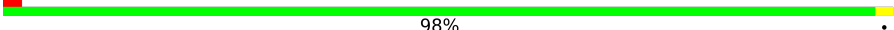

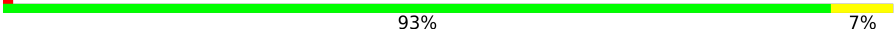


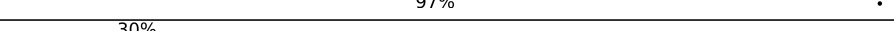


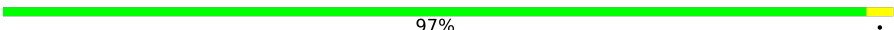
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Mol	Chain	Length	Quality of chain
3	2D	275	% 97% .
4	1E	204	% 99% .
4	2E	204	5% 97% .
5	1F	203	% 96% .
5	2F	203	3% 96% .
6	1G	181	16% 96% .
6	2G	181	30% 93% 7%
7	1H	174	97% .
7	2H	174	18% 93% 6% .
8	1I	147	11% 92% 8%
8	2I	147	14% 92% 7% .
9	1N	140	97% .
9	2N	140	% 94% 6%
10	1O	122	97% .
10	2O	122	% 94% 6%
11	1P	149	97% .
11	2P	149	6% 95% 5%
12	1Q	141	93% 6% .
12	2Q	141	% 95% 5%
13	1R	118	97% .
13	2R	118	92% 8%
14	1S	110	3% 96% .
14	2S	110	15% 96% .
15	1T	131	92% 7% .
15	2T	131	2% 96% . .

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Mol	Chain	Length	Quality of chain
16	1U	116	 99%
16	2U	116	 3% 96%
17	1V	101	 96%
17	2V	101	 5% 96%
18	1W	112	 % 95%
18	2W	112	 % 89% 11%
19	1X	95	 96%
19	2X	95	 % 94% 6%
20	1Y	107	 2% 94% 6%
20	2Y	107	 9% 97%
21	1Z	203	 93% 7%
21	2Z	203	 11% 91% 8%
22	10	77	 % 96%
22	20	77	 4% 96%
23	11	97	 98%
23	21	97	 2% 98%
24	12	70	 % 96%
24	22	70	 % 93% 7%
25	13	59	 98%
25	23	59	 7% 97%
26	14	69	 30% 90% 9%
26	24	69	 46% 91% 9%
27	15	59	 97%
27	25	59	 2% 100%
28	16	53	 94% 6%

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Mol	Chain	Length	Quality of chain
28	26	53	 6% 100%
29	17	48	 2% 96% .
29	27	48	 98% .
30	18	64	 98% .
30	28	64	 100%
31	19	37	 100%
31	29	37	 8% 97% .
32	1a	2331	 14% 52% 12% 36%
32	2a	2331	 15% 52% 12% 35%
33	1b	231	 13% 86% 13% .
33	2b	231	 18% 91% 9%
34	1c	206	 33% 95% 5%
34	2c	206	 33% 94% 6%
35	1d	208	 12% 93% 7%
35	2d	208	 10% 96% .
36	1e	148	 7% 95% 5%
36	2e	148	 9% 95% 5%
37	1f	100	 5% 97% .
37	2f	100	 9% 96% . .
38	1g	155	 40% 96% .
38	2g	155	 41% 93% 7%
39	1h	137	 % 93% 7%
39	2h	137	 4% 92% 8%
40	1i	127	 51% 94% 6%
40	2i	127	 39% 93% 6% . .

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Mol	Chain	Length	Quality of chain
41	1j	97	<div> <div>55%</div> <div>93%</div> <div>7%</div> </div>
41	2j	97	<div> <div>44%</div> <div>93%</div> <div>6%</div> </div>
42	1k	114	<div> <div>12%</div> <div>94%</div> <div>6%</div> </div>
42	2k	114	<div> <div>25%</div> <div>93%</div> <div>7%</div> </div>
43	1l	122	<div> <div></div> <div>92%</div> <div>8%</div> </div>
43	2l	122	<div> <div>3%</div> <div>97%</div> <div></div> </div>
44	1m	116	<div> <div>49%</div> <div>97%</div> <div></div> </div>
44	2m	116	<div> <div>39%</div> <div>93%</div> <div>5%</div> </div>
45	1n	60	<div> <div>23%</div> <div>93%</div> <div>7%</div> </div>
45	2n	60	<div> <div>18%</div> <div>90%</div> <div>10%</div> </div>
46	1o	88	<div> <div>5%</div> <div>88%</div> <div>13%</div> </div>
46	2o	88	<div> <div>6%</div> <div>91%</div> <div>9%</div> </div>
47	1p	82	<div> <div>15%</div> <div>96%</div> <div></div> </div>
47	2p	82	<div> <div>9%</div> <div>94%</div> <div>6%</div> </div>
48	1q	99	<div> <div>17%</div> <div>96%</div> <div></div> </div>
48	2q	99	<div> <div>15%</div> <div>96%</div> <div></div> </div>
49	1r	68	<div> <div>6%</div> <div>90%</div> <div>9%</div> </div>
49	2r	68	<div> <div>9%</div> <div>91%</div> <div>9%</div> </div>
50	1s	83	<div> <div>59%</div> <div>96%</div> <div>...</div> </div>
50	2s	83	<div> <div>52%</div> <div>94%</div> <div>6%</div> </div>
51	1t	98	<div> <div>6%</div> <div>93%</div> <div>5%</div> </div>
51	2t	98	<div> <div>%</div> <div>90%</div> <div>10%</div> </div>
52	1u	23	<div> <div>61%</div> <div>87%</div> <div>13%</div> </div>
52	2u	23	<div> <div>61%</div> <div>87%</div> <div>13%</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	2MG	1a	1189	-	-	-	X
53	MG	1A	3002	-	-	-	X
53	MG	1A	3042	-	-	-	X
53	MG	1A	3044	-	-	-	X
53	MG	1A	3049	-	-	-	X
53	MG	1A	3055	-	-	-	X
53	MG	1A	3097	-	-	-	X
53	MG	1A	3114	-	-	-	X
53	MG	1A	3124	-	-	-	X
53	MG	1A	3129	-	-	-	X
53	MG	1A	3130	-	-	-	X
53	MG	1A	3154	-	-	-	X
53	MG	1A	3165	-	-	-	X
53	MG	1A	3188	-	-	-	X
53	MG	1A	3293	-	-	-	X
53	MG	1A	3296	-	-	-	X
53	MG	1A	3325	-	-	-	X
53	MG	1A	3388	-	-	-	X
53	MG	1A	3402	-	-	-	X
53	MG	1A	3413	-	-	-	X
53	MG	1A	3466	-	-	-	X
53	MG	1A	3473	-	-	-	X
53	MG	1A	3478	-	-	-	X
53	MG	1A	3482	-	-	-	X
53	MG	1A	3493	-	-	-	X
53	MG	1A	3525	-	-	-	X
53	MG	1A	3530	-	-	-	X
53	MG	1A	3531	-	-	-	X
53	MG	1A	3542	-	-	-	X
53	MG	1A	3545	-	-	-	X
53	MG	1A	3548	-	-	-	X
53	MG	1A	3555	-	-	-	X
53	MG	1A	3557	-	-	-	X
53	MG	1A	3600	-	-	-	X
53	MG	1A	3601	-	-	-	X
53	MG	1A	3606	-	-	-	X
53	MG	1A	3630	-	-	-	X
53	MG	1A	3632	-	-	-	X
53	MG	1A	3639	-	-	-	X
53	MG	1A	3665	-	-	-	X
53	MG	1A	3712	-	-	-	X
53	MG	1A	3741	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
53	MG	1A	3752	-	-	-	X
53	MG	1A	3769	-	-	-	X
53	MG	1A	3772	-	-	-	X
53	MG	1A	3777	-	-	-	X
53	MG	1A	3781	-	-	-	X
53	MG	1B	213	-	-	-	X
53	MG	1B	221	-	-	-	X
53	MG	1B	225	-	-	-	X
53	MG	1D	303	-	-	-	X
53	MG	1F	306	-	-	-	X
53	MG	1Q	202	-	-	-	X
53	MG	1T	8002	-	-	-	X
53	MG	1W	3002	-	-	-	X
53	MG	1a	1714	-	-	-	X
53	MG	1a	1716	-	-	-	X
53	MG	1a	1717	-	-	-	X
53	MG	1a	1727	-	-	-	X
53	MG	1a	1733	-	-	-	X
53	MG	1a	1735	-	-	-	X
53	MG	1a	1736	-	-	-	X
53	MG	1a	1744	-	-	-	X
53	MG	1a	1748	-	-	-	X
53	MG	1a	1753	-	-	-	X
53	MG	1a	1754	-	-	-	X
53	MG	1a	1770	-	-	-	X
53	MG	1a	1781	-	-	-	X
53	MG	1a	1784	-	-	-	X
53	MG	1a	1785	-	-	-	X
53	MG	1a	1801	-	-	-	X
53	MG	1a	1810	-	-	-	X
53	MG	1a	1819	-	-	-	X
53	MG	1a	1821	-	-	-	X
53	MG	1a	1845	-	-	-	X
53	MG	1a	1846	-	-	-	X
53	MG	1a	1847	-	-	-	X
53	MG	1a	1851	-	-	-	X
53	MG	1a	1852	-	-	-	X
53	MG	1a	1854	-	-	-	X
53	MG	1a	1857	-	-	-	X
53	MG	1a	1858	-	-	-	X
53	MG	1a	1865	-	-	-	X
53	MG	1a	1867	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
53	MG	1a	1872	-	-	-	X
53	MG	1a	1881	-	-	-	X
53	MG	1a	1891	-	-	-	X
53	MG	1h	3001	-	-	-	X
53	MG	1m	201	-	-	-	X
53	MG	1t	3001	-	-	-	X
53	MG	28	8002	-	-	-	X
53	MG	2A	3005	-	-	-	X
53	MG	2A	3010	-	-	-	X
53	MG	2A	3024	-	-	-	X
53	MG	2A	3032	-	-	-	X
53	MG	2A	3035	-	-	-	X
53	MG	2A	3037	-	-	-	X
53	MG	2A	3061	-	-	-	X
53	MG	2A	3068	-	-	-	X
53	MG	2A	3070	-	-	-	X
53	MG	2A	3084	-	-	-	X
53	MG	2A	3087	-	-	-	X
53	MG	2A	3088	-	-	-	X
53	MG	2A	3098	-	-	-	X
53	MG	2A	3103	-	-	-	X
53	MG	2A	3117	-	-	-	X
53	MG	2A	3128	-	-	-	X
53	MG	2A	3139	-	-	-	X
53	MG	2A	3158	-	-	-	X
53	MG	2A	3173	-	-	-	X
53	MG	2A	3185	-	-	-	X
53	MG	2A	3197	-	-	-	X
53	MG	2A	3205	-	-	-	X
53	MG	2A	3212	-	-	-	X
53	MG	2A	3219	-	-	-	X
53	MG	2A	3230	-	-	-	X
53	MG	2A	3236	-	-	-	X
53	MG	2A	3284	-	-	-	X
53	MG	2A	3290	-	-	-	X
53	MG	2A	3325	-	-	-	X
53	MG	2A	3348	-	-	-	X
53	MG	2A	3367	-	-	-	X
53	MG	2A	3368	-	-	-	X
53	MG	2A	3376	-	-	-	X
53	MG	2A	3407	-	-	-	X
53	MG	2A	3460	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
53	MG	2A	3469	-	-	-	X
53	MG	2A	3485	-	-	-	X
53	MG	2A	3495	-	-	-	X
53	MG	2A	3500	-	-	-	X
53	MG	2A	3510	-	-	-	X
53	MG	2A	3518	-	-	-	X
53	MG	2A	3525	-	-	-	X
53	MG	2A	3539	-	-	-	X
53	MG	2A	3543	-	-	-	X
53	MG	2A	3546	-	-	-	X
53	MG	2B	206	-	-	-	X
53	MG	2D	307	-	-	-	X
53	MG	2O	202	-	-	-	X
53	MG	2P	202	-	-	-	X
53	MG	2X	101	-	-	-	X
53	MG	2a	1703	-	-	-	X
53	MG	2a	1707	-	-	-	X
53	MG	2a	1713	-	-	-	X
53	MG	2a	1722	-	-	-	X
53	MG	2a	1727	-	-	-	X
53	MG	2a	1732	-	-	-	X
53	MG	2a	1737	-	-	-	X
53	MG	2a	1738	-	-	-	X
53	MG	2a	1740	-	-	-	X
53	MG	2a	1743	-	-	-	X
53	MG	2a	1744	-	-	-	X
53	MG	2a	1755	-	-	-	X
53	MG	2a	1757	-	-	-	X
53	MG	2a	1758	-	-	-	X
53	MG	2a	1759	-	-	-	X
53	MG	2a	1767	-	-	-	X
53	MG	2a	1769	-	-	-	X
53	MG	2a	1774	-	-	-	X
53	MG	2a	1777	-	-	-	X
53	MG	2a	1783	-	-	-	X
53	MG	2a	1786	-	-	-	X
53	MG	2a	1789	-	-	-	X
53	MG	2a	1794	-	-	-	X
53	MG	2a	1801	-	-	-	X
53	MG	2a	1804	-	-	-	X
53	MG	2a	1812	-	-	-	X
53	MG	2a	1818	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
53	MG	2a	1832	-	-	-	X
53	MG	2a	1833	-	-	-	X
53	MG	2a	1837	-	-	-	X
53	MG	2a	1840	-	-	-	X
53	MG	2h	201	-	-	-	X
53	MG	2n	101	-	-	-	X
53	MG	2r	101	-	-	-	X
55	MPD	2B	210	-	-	-	X

## 2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 290633 atoms, of which 88 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	2872	Total	C	N	O	P	0	0	0
			61868	27540	11574	19883	2871			
1	2A	2867	Total	C	N	O	P	0	0	0
			61758	27491	11552	19850	2865			

- 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
			2572	1145	476	832	119			
2	2B	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

- 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
			2131	1346	422	360	3			
3	2D	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	1F	203	Total	C	N	O	S	0	0	1
			1584	1009	298	275	2			
5	2F	203	Total	C	N	O	S	0	0	1
			1580	1007	297	274	2			

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	1G	181	Total	C	N	O	S	0	0	0
			1426	916	253	253	4			
6	2G	181	Total	C	N	O	S	0	0	0
			1424	912	259	249	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	173	Total	C	N	O	S	0	0	0
			1324	842	247	234	1			

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	1I	147	Total	C	N	O	S	0	0	0
			1094	699	191	203	1			
8	2I	146	Total	C	N	O	S	0	0	0
			1080	690	187	202	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
			1121	722	208	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
			877	553	175	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
			775	498	141	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
			810	520	153	131	6			
20	2Y	107	Total	C	N	O	S	0	0	0
			810	519	153	132	6			

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	1Z	203	Total	C	N	O	S	0	0	0
			1587	1011	282	292	2			
21	2Z	201	Total	C	N	O	S	0	0	0
			1557	995	274	286	2			

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	10	77	Total	C	N	O	S	0	0	0
			608	375	129	103	1			
22	20	77	Total	C	N	O	S	0	0	0
			608	375	129	103	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
			754	475	148	130	1			
23	21	97	Total	C	N	O	S	0	0	0
			759	478	149	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
			592	368	119	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
			546	346	96	99	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	24	69	Total	C	N	O	S	0	0	0
			536	342	98	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
			459	288	90	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	1504	Total	C	N	O	P	0	0	0
			32331	14396	5990	10441	1504			

- 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
			1842	1175	330	332	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
			1558	979	305	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
			1665	1043	329	286	7			
35	2d	208	Total	C	N	O	S	0	0	0
			1668	1047	330	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
			1133	716	214	199	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
			814	516	144	151	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
			1235	769	244	216	6			
38	2g	155	Total	C	N	O	S	0	0	0
			1229	766	241	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
			1098	694	210	192	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
			986	625	193	168			
40	2i	126	Total	C	N	O	0	0	0
			966	613	186	167			

- 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
			719	446	142	131			
41	2j	96	Total	C	N	O	0	0	0
			710	442	137	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
			834	520	156	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	116	Total	C	N	O	S	0	0	0
			914	564	189	159	2			
44	2m	114	Total	C	N	O	S	0	0	0
			895	550	186	157	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
			648	415	120	111	2			
50	2s	83	Total	C	N	O	S	0	0	0
			645	410	118	115	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
			732	449	157	124	2			
51	2t	98	Total	C	N	O	S	0	0	0
			733	451	154	126	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 MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
53	2E	5	Total Mg 5 5	0	0
53	17	3	Total Mg 3 3	0	0
53	1T	3	Total Mg 3 3	0	0
53	1N	4	Total Mg 4 4	0	0
53	20	1	Total Mg 1 1	0	0
53	18	3	Total Mg 3 3	0	0
53	1o	1	Total Mg 1 1	0	0
53	2W	2	Total Mg 2 2	0	0
53	1Y	1	Total Mg 1 1	0	0
53	2I	2	Total Mg 2 2	0	0
53	13	1	Total Mg 1 1	0	0
53	1f	2	Total Mg 2 2	0	0
53	2h	1	Total Mg 1 1	0	0
53	1P	3	Total Mg 3 3	0	0
53	2B	9	Total Mg 9 9	0	0
53	2a	144	Total Mg 144 144	0	0
53	1E	9	Total Mg 9 9	0	0
53	1b	1	Total Mg 1 1	0	0
53	2I	2	Total Mg 2 2	0	0
53	2F	4	Total Mg 4 4	0	0
53	28	4	Total Mg 4 4	0	0
53	2e	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
53	1W	2	Total 2	Mg 2	0	0
53	1A	837	Total 837	Mg 837	0	0
53	1t	1	Total 1	Mg 1	0	0
53	2P	3	Total 3	Mg 3	0	0
53	1X	1	Total 1	Mg 1	0	0
53	1S	1	Total 1	Mg 1	0	0
53	25	1	Total 1	Mg 1	0	0
53	2T	3	Total 3	Mg 3	0	0
53	1D	15	Total 15	Mg 15	0	0
53	1e	1	Total 1	Mg 1	0	0
53	2G	1	Total 1	Mg 1	0	0
53	2f	2	Total 2	Mg 2	0	0
53	1V	3	Total 3	Mg 3	0	0
53	2X	1	Total 1	Mg 1	0	0
53	1a	203	Total 203	Mg 203	0	0
53	2Q	1	Total 1	Mg 1	0	0
53	15	1	Total 1	Mg 1	0	0
53	1R	3	Total 3	Mg 3	0	0
53	1s	1	Total 1	Mg 1	0	0
53	1m	1	Total 1	Mg 1	0	0
53	2U	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
53	1G	3	Total 3	Mg 3	0	0
53	2O	2	Total 2	Mg 2	0	0
53	11	3	Total 3	Mg 3	0	0
53	1d	2	Total 2	Mg 2	0	0
53	2n	1	Total 1	Mg 1	0	0
53	1H	3	Total 3	Mg 3	0	0
53	21	1	Total 1	Mg 1	0	0
53	2Y	1	Total 1	Mg 1	0	0
53	2R	2	Total 2	Mg 2	0	0
53	1Z	2	Total 2	Mg 2	0	0
53	2D	7	Total 7	Mg 7	0	0
53	1U	1	Total 1	Mg 1	0	0
53	2r	2	Total 2	Mg 2	0	0
53	1O	1	Total 1	Mg 1	0	0
53	27	1	Total 1	Mg 1	0	0
53	19	2	Total 2	Mg 2	0	0
53	1l	2	Total 2	Mg 2	0	0
53	2V	1	Total 1	Mg 1	0	0
53	1F	9	Total 9	Mg 9	0	0
53	10	6	Total 6	Mg 6	0	0
53	2t	1	Total 1	Mg 1	0	0

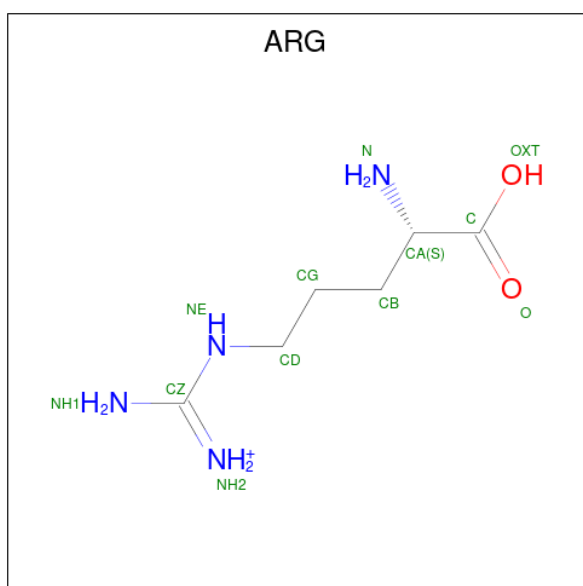
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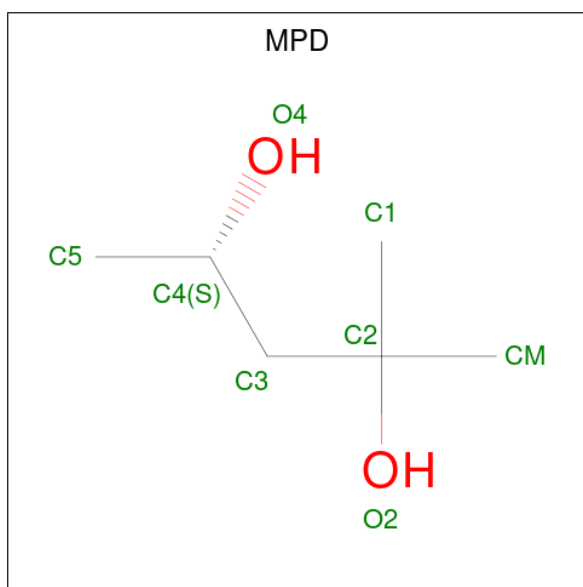
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
53	1Q	3	Total	Mg	0	0
			3	3		
53	2A	561	Total	Mg	0	0
			561	561		
53	1h	1	Total	Mg	0	0
			1	1		
53	2Z	1	Total	Mg	0	0
			1	1		
53	1B	24	Total	Mg	0	0
			24	24		

- Molecule 54 is ARGinine (three-letter code: ARG) (formula:  $C_6H_{15}N_4O_2$ ).



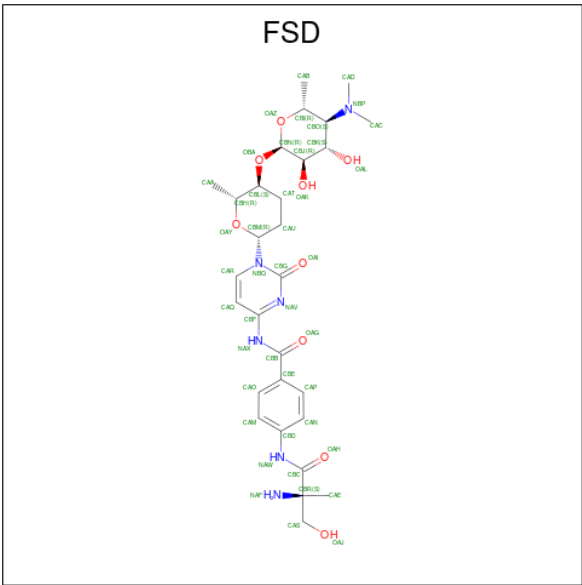
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
54	1A	1	Total	C	N	O	0	0
			12	6	4	2		
54	1B	1	Total	C	N	O	0	0
			12	6	4	2		

- Molecule 55 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
55	1A	1	Total	C	O	0	0
			8	6	2		
55	1T	1	Total	C	O	0	0
			8	6	2		
55	18	1	Total	C	O	0	0
			8	6	2		
55	1a	1	Total	C	O	0	0
			8	6	2		
55	2A	1	Total	C	O	0	0
			8	6	2		
55	2A	1	Total	C	O	0	0
			8	6	2		
55	2B	1	Total	C	O	0	0
			8	6	2		

- Molecule 56 is amicetin (three-letter code: FSD) (formula:  $C_{29}H_{42}N_6O_9$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
56	1A	1	Total	C	H	N	O	0	0
			88	29	44	6	9		
56	2A	1	Total	C	H	N	O	0	0
			88	29	44	6	9		

- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	19	1	Total	Zn	0	0
			1	1		
57	15	1	Total	Zn	0	0
			1	1		
57	29	1	Total	Zn	0	0
			1	1		
57	1Y	1	Total	Zn	0	0
			1	1		
57	26	1	Total	Zn	0	0
			1	1		
57	25	1	Total	Zn	0	0
			1	1		
57	2n	1	Total	Zn	0	0
			1	1		
57	2Y	1	Total	Zn	0	0
			1	1		
57	16	1	Total	Zn	0	0
			1	1		

- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	1d	1	Total	Fe	S	0	0
			8	4	4		
58	2d	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 59 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1A	1757	Total	O	0	0
			1757	1757		
59	1B	40	Total	O	0	0
			40	40		
59	1D	49	Total	O	0	0
			49	49		
59	1E	31	Total	O	0	0
			31	31		
59	1F	32	Total	O	0	0
			32	32		
59	1G	6	Total	O	0	0
			6	6		
59	1H	10	Total	O	0	0
			10	10		
59	1I	2	Total	O	0	0
			2	2		
59	1N	34	Total	O	0	0
			34	34		
59	1O	10	Total	O	0	0
			10	10		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1P	28	Total 28	O 28	0	0
59	1Q	19	Total 19	O 19	0	0
59	1R	18	Total 18	O 18	0	0
59	1S	3	Total 3	O 3	0	0
59	1T	14	Total 14	O 14	0	0
59	1U	24	Total 24	O 24	0	0
59	1V	33	Total 33	O 33	0	0
59	1W	21	Total 21	O 21	0	0
59	1X	5	Total 5	O 5	0	0
59	1Y	7	Total 7	O 7	0	0
59	1Z	6	Total 6	O 6	0	0
59	10	16	Total 16	O 16	0	0
59	11	13	Total 13	O 13	0	0
59	12	5	Total 5	O 5	0	0
59	13	8	Total 8	O 8	0	0
59	15	6	Total 6	O 6	0	0
59	16	5	Total 5	O 5	0	0
59	17	3	Total 3	O 3	0	0
59	18	18	Total 18	O 18	0	0
59	19	9	Total 9	O 9	0	0
59	1a	235	Total 235	O 235	0	0

*Continued on next page...*

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1c	1	Total 1	O 1	0	0
59	1d	4	Total 4	O 4	0	0
59	1e	1	Total 1	O 1	0	0
59	1h	2	Total 2	O 2	0	0
59	1i	1	Total 1	O 1	0	0
59	1l	2	Total 2	O 2	0	0
59	1m	1	Total 1	O 1	0	0
59	1o	2	Total 2	O 2	0	0
59	1q	1	Total 1	O 1	0	0
59	2A	859	Total 859	O 859	0	0
59	2B	5	Total 5	O 5	0	0
59	2D	12	Total 12	O 12	0	0
59	2E	11	Total 11	O 11	0	0
59	2F	6	Total 6	O 6	0	0
59	2G	4	Total 4	O 4	0	0
59	2I	1	Total 1	O 1	0	0
59	2O	6	Total 6	O 6	0	0
59	2P	7	Total 7	O 7	0	0
59	2Q	5	Total 5	O 5	0	0
59	2R	5	Total 5	O 5	0	0
59	2S	1	Total 1	O 1	0	0

*Continued on next page...*

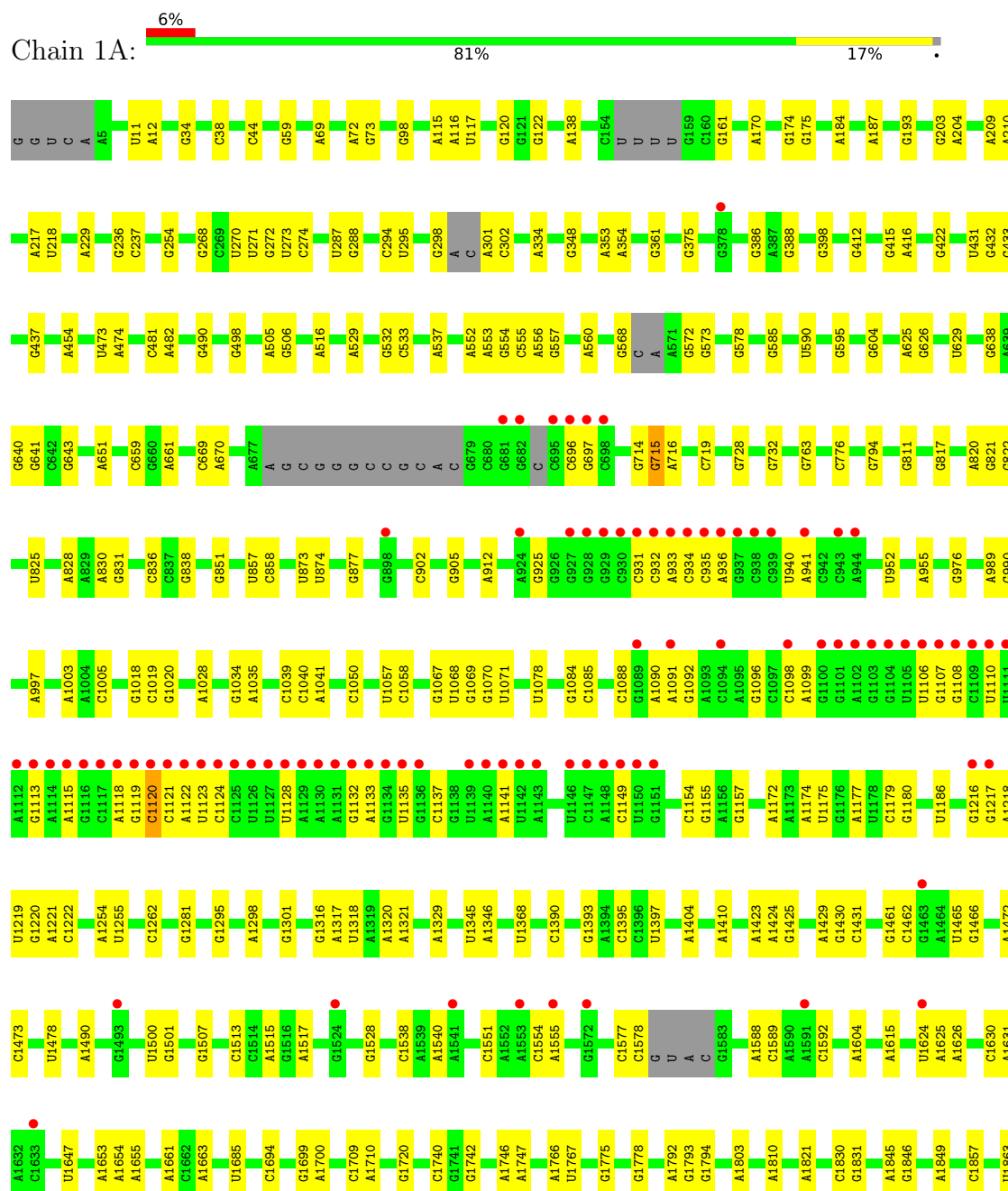
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	2T	4	Total 4	O 4	0	0
59	2U	5	Total 5	O 5	0	0
59	2V	3	Total 3	O 3	0	0
59	2W	4	Total 4	O 4	0	0
59	2X	5	Total 5	O 5	0	0
59	2Y	2	Total 2	O 2	0	0
59	20	5	Total 5	O 5	0	0
59	21	4	Total 4	O 4	0	0
59	22	1	Total 1	O 1	0	0
59	23	2	Total 2	O 2	0	0
59	25	1	Total 1	O 1	0	0
59	26	2	Total 2	O 2	0	0
59	27	5	Total 5	O 5	0	0
59	28	5	Total 5	O 5	0	0
59	2a	113	Total 113	O 113	0	0
59	2f	1	Total 1	O 1	0	0
59	2o	1	Total 1	O 1	0	0
59	2q	1	Total 1	O 1	0	0

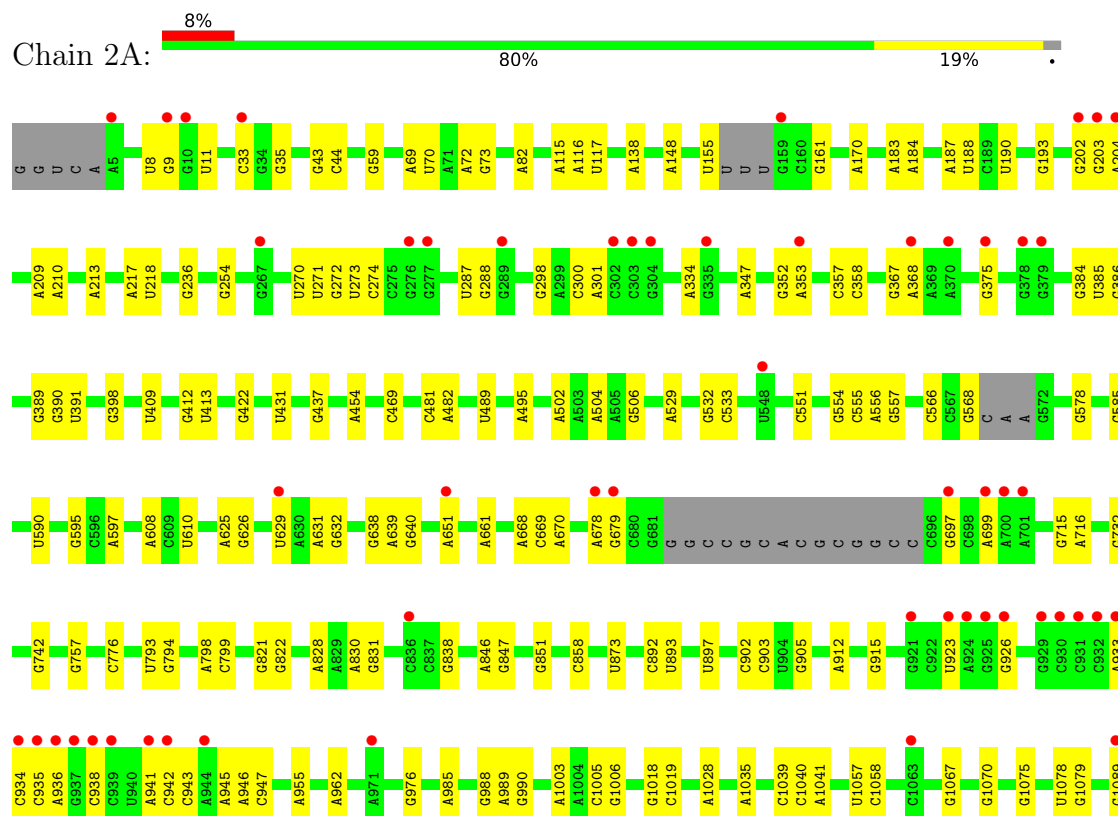
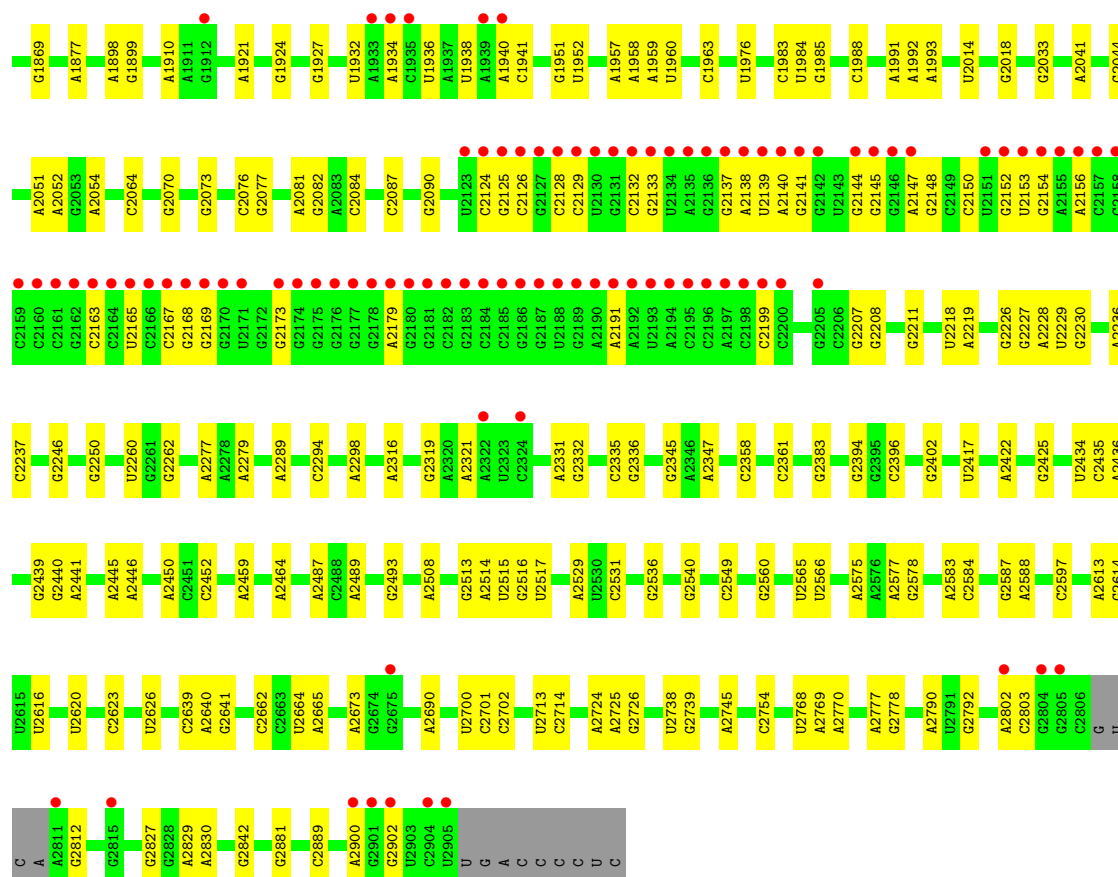
### 3 Residue-property plots

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

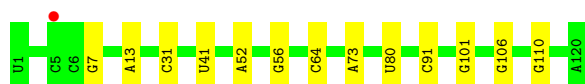
#### • Molecule 1: 23S Ribosomal RNA



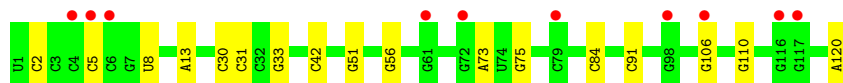
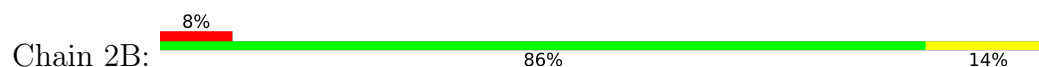








- Molecule 2: 5S Ribosomal RNA



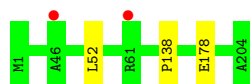
- Molecule 3: 50S ribosomal protein L2



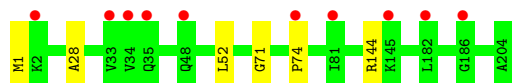
- Molecule 3: 50S ribosomal protein L2



- Molecule 4: 50S ribosomal protein L3



- Molecule 4: 50S ribosomal protein L3



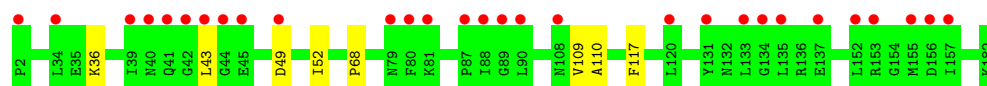
- Molecule 5: 50S ribosomal protein L4



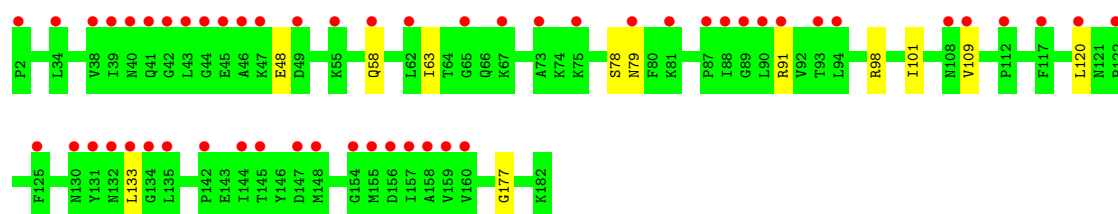
- Molecule 5: 50S ribosomal protein L4



- Molecule 6: 50S ribosomal protein L5



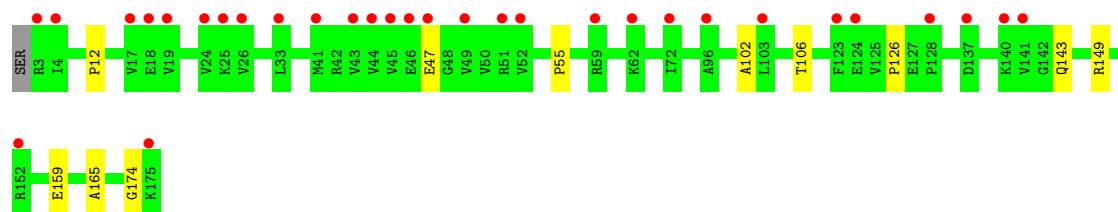
- Molecule 6: 50S ribosomal protein L5



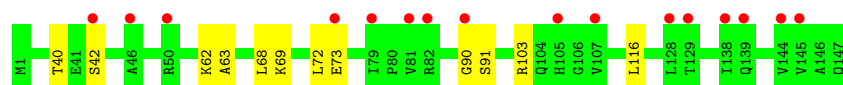
- Molecule 7: 50S ribosomal protein L6



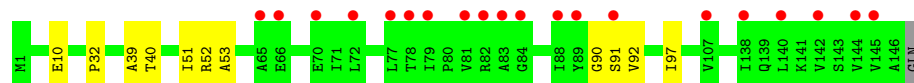
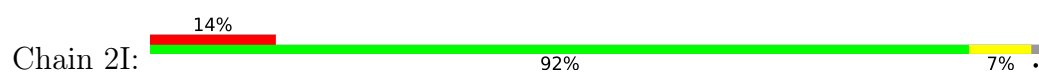
- Molecule 7: 50S ribosomal protein L6



- 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



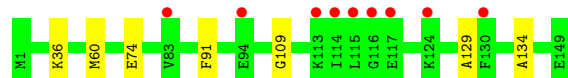
- Molecule 10: 50S ribosomal protein L14



- Molecule 11: 50S ribosomal protein L15



- Molecule 11: 50S ribosomal protein L15



- Molecule 12: 50S ribosomal protein L16

Chain 1Q:  93% 6% .



- Molecule 12: 50S ribosomal protein L16

Chain 2Q:  95% 5% .



- Molecule 13: 50S ribosomal protein L17

Chain 1R:  97% .



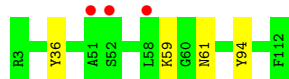
- Molecule 13: 50S ribosomal protein L17

Chain 2R:  92% 8% .



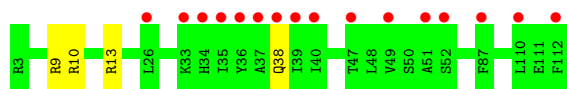
- Molecule 14: 50S ribosomal protein L18

Chain 1S:  96% .



- Molecule 14: 50S ribosomal protein L18

Chain 2S:  96% .

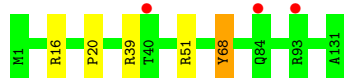


- Molecule 15: 50S ribosomal protein L19

Chain 1T:  92% 7% .



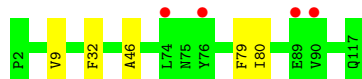
- Molecule 15: 50S ribosomal protein L19



- Molecule 16: 50S ribosomal protein L20



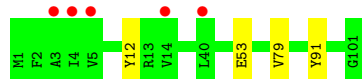
- Molecule 16: 50S ribosomal protein L20



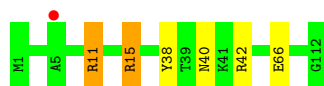
- Molecule 17: 50S ribosomal protein L21



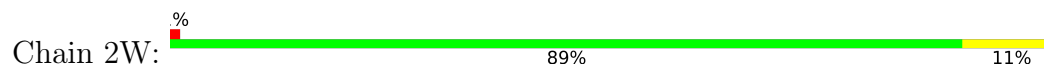
- Molecule 17: 50S ribosomal protein L21



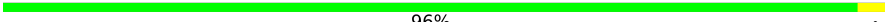
- Molecule 18: 50S ribosomal protein L22

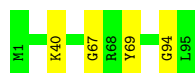


- Molecule 18: 50S ribosomal protein L22



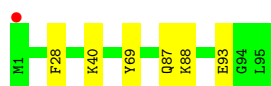
- Molecule 19: 50S ribosomal protein L23

Chain 1X:  96% .



- Molecule 19: 50S ribosomal protein L23

Chain 2X:  94% 6%



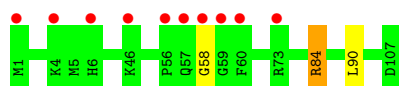
- Molecule 20: 50S ribosomal protein L24

Chain 1Y:  94% 6%



- Molecule 20: 50S ribosomal protein L24

Chain 2Y:  97% ..



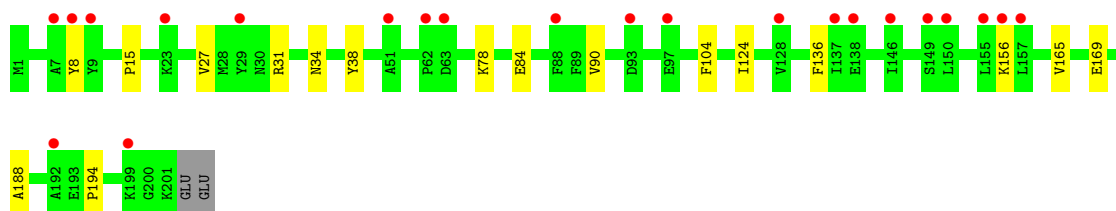
- Molecule 21: 50S ribosomal protein L25

Chain 1Z:  93% 7%



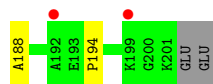
- Molecule 21: 50S ribosomal protein L25

Chain 2Z:  91% 8% .



- Molecule 22: 50S ribosomal protein L27

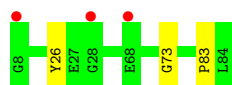
Chain 10:  96% .







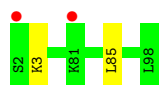
- Molecule 22: 50S ribosomal protein L27



- Molecule 23: 50S ribosomal protein L28



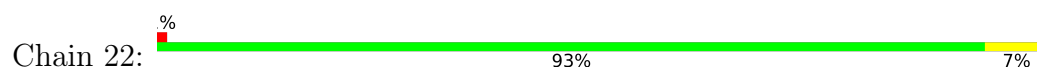
- Molecule 23: 50S ribosomal protein L28



- Molecule 24: 50S ribosomal protein L29



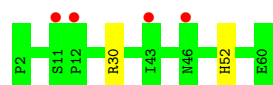
- Molecule 24: 50S ribosomal protein L29



- Molecule 25: 50S ribosomal protein L30



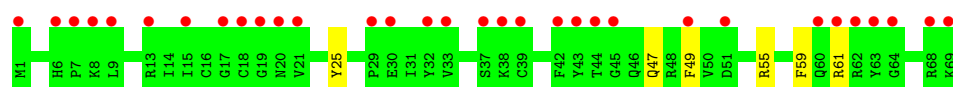
- Molecule 25: 50S ribosomal protein L30



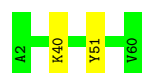
- Molecule 26: 50S ribosomal protein L31



- Molecule 26: 50S ribosomal protein L31



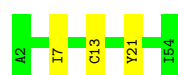
- Molecule 27: 50S ribosomal protein L32



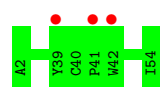
- Molecule 27: 50S ribosomal protein L32



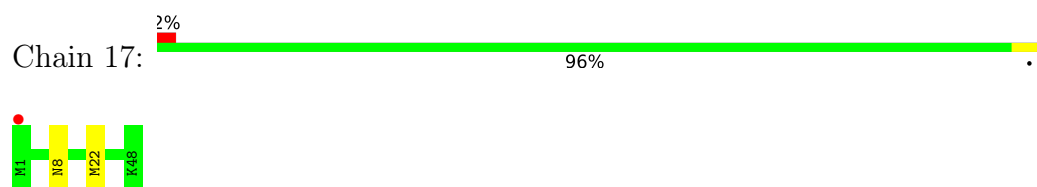
- Molecule 28: 50S ribosomal protein L33



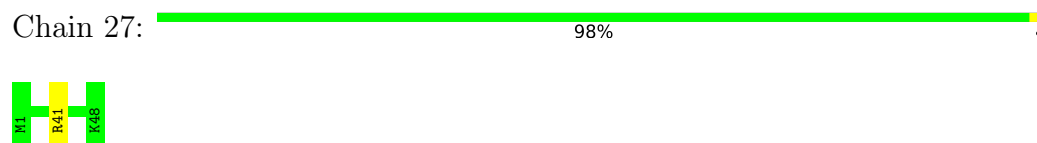
- Molecule 28: 50S ribosomal protein L33



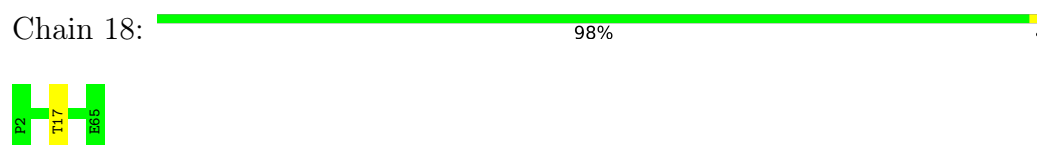
- Molecule 29: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L34



- Molecule 30: 50S ribosomal protein L35



- Molecule 30: 50S ribosomal protein L35



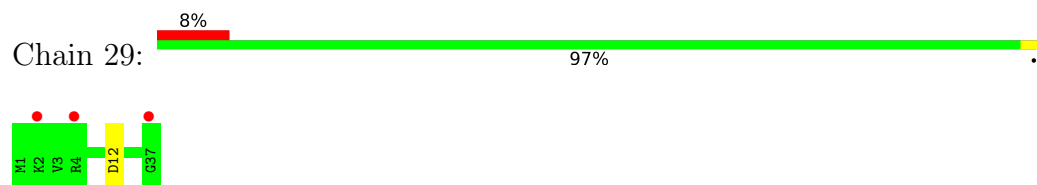
There are no outlier residues recorded for this chain.

- Molecule 31: 50S ribosomal protein L36

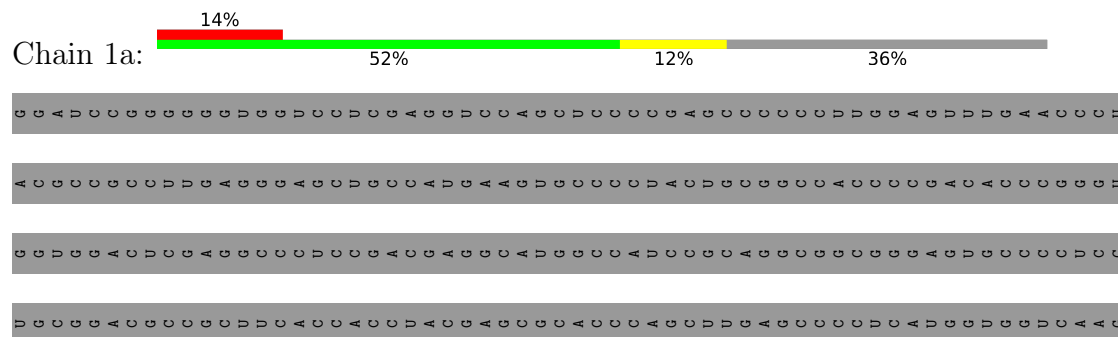


There are no outlier residues recorded for this chain.

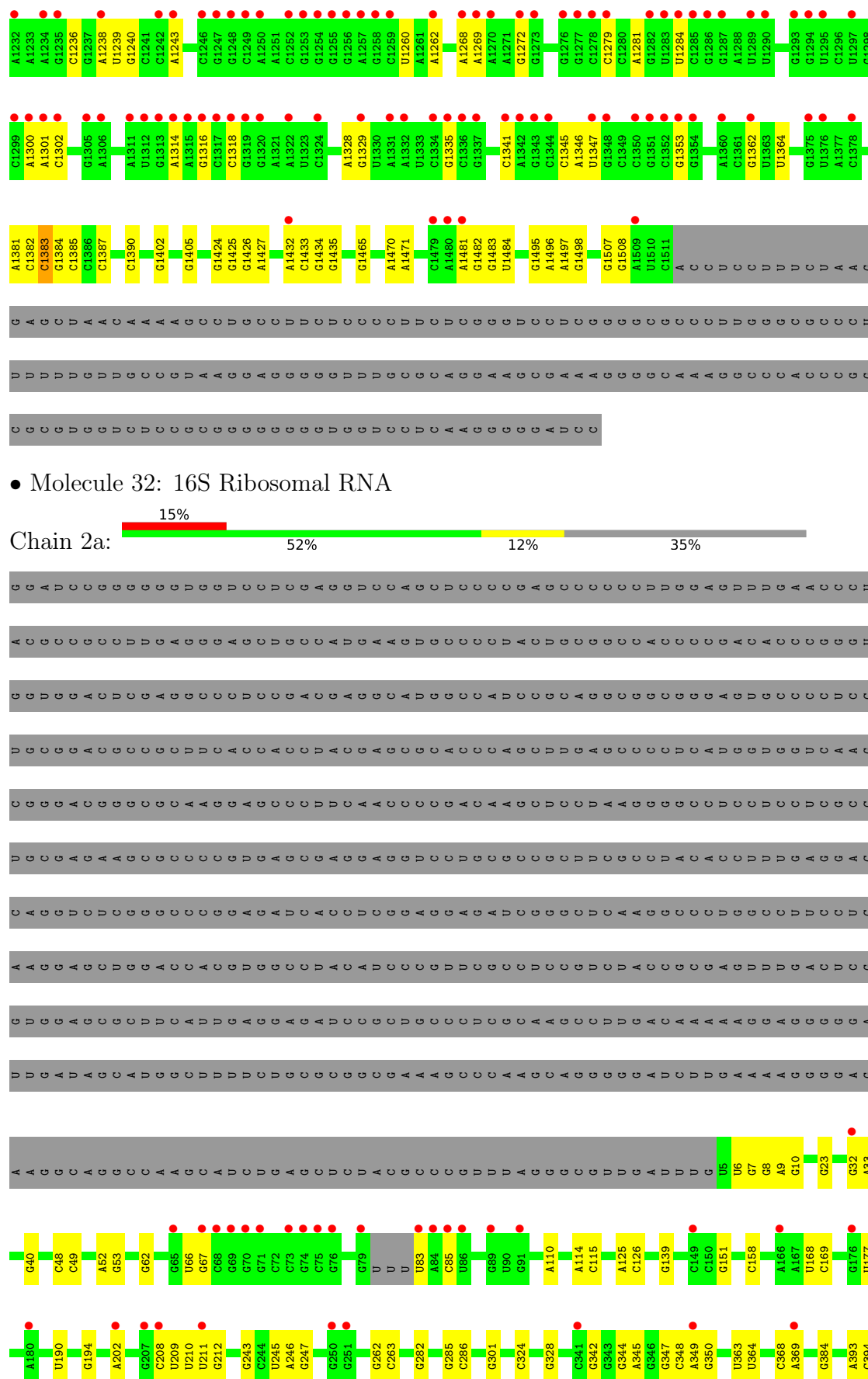
- Molecule 31: 50S ribosomal protein L36

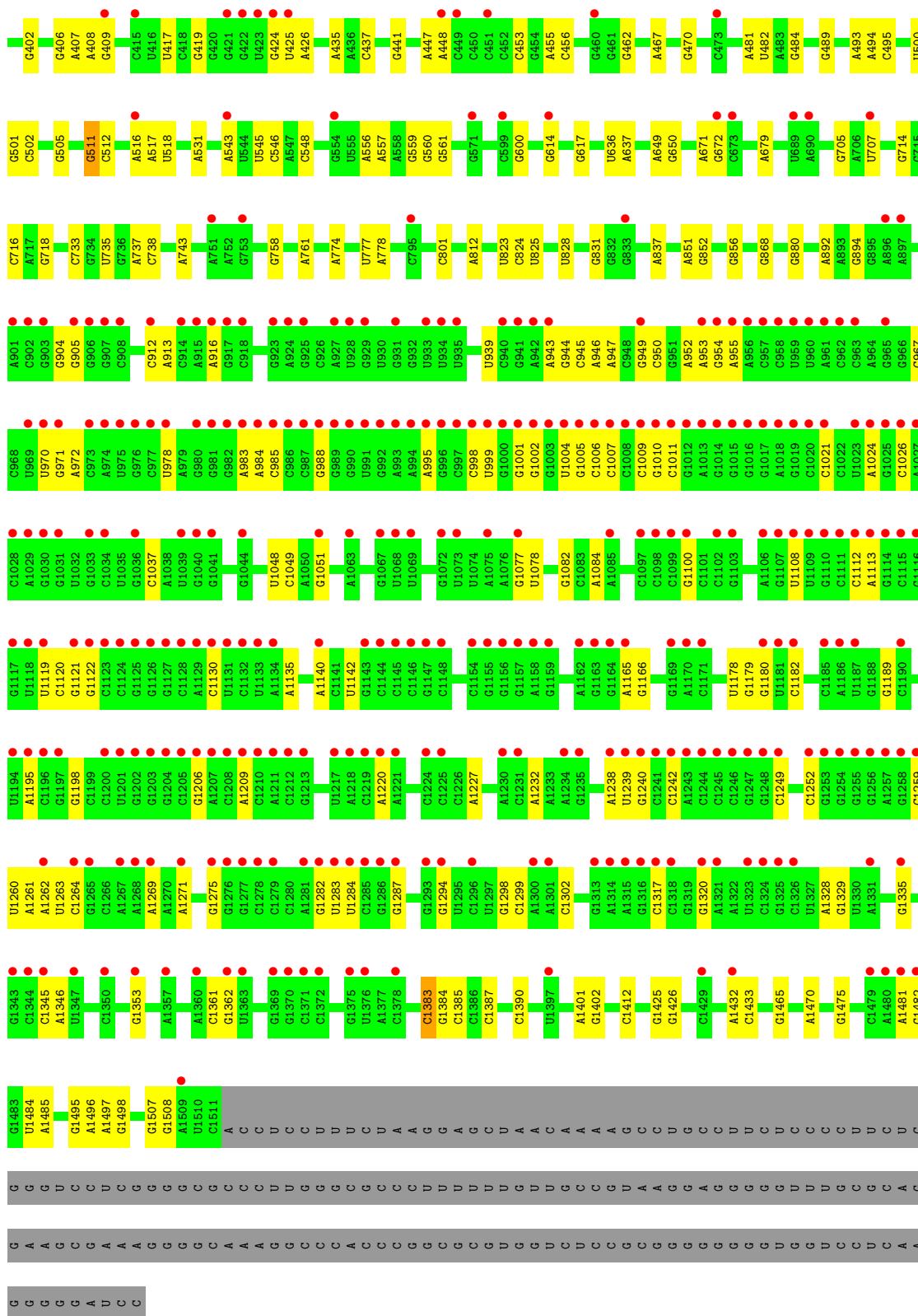


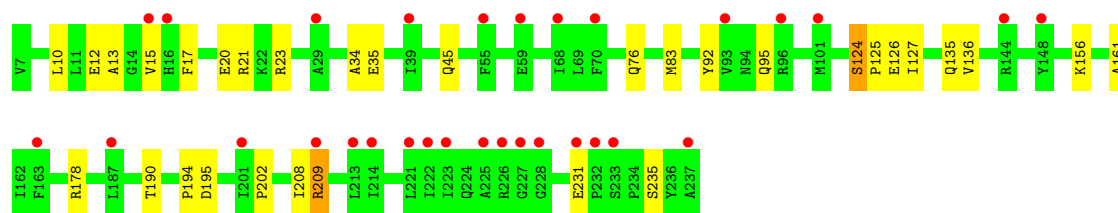
- Molecule 32: 16S Ribosomal RNA



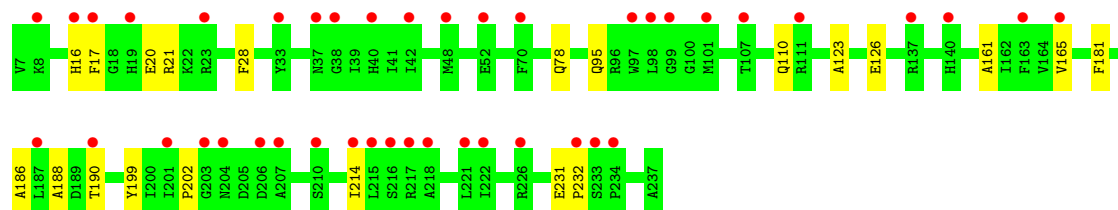
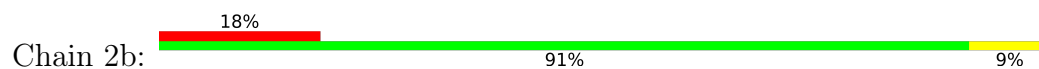




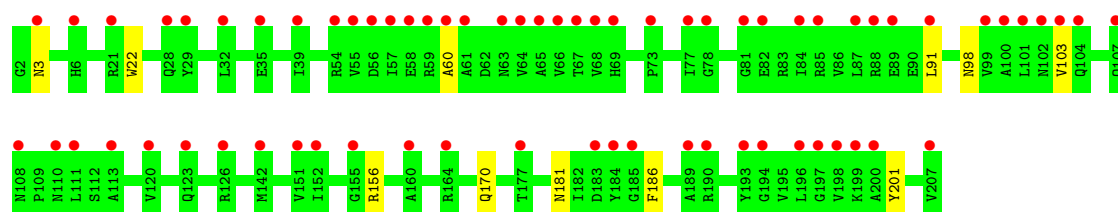




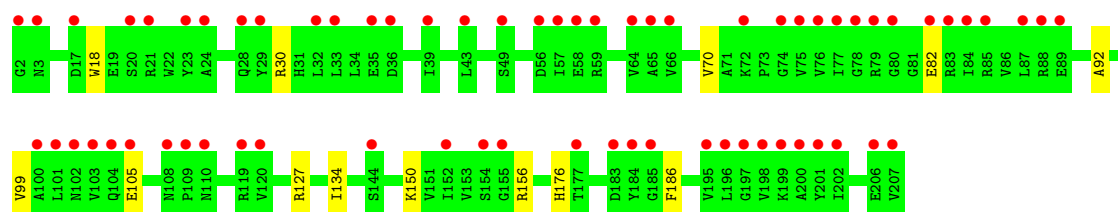
• Molecule 33: 30S ribosomal protein S2



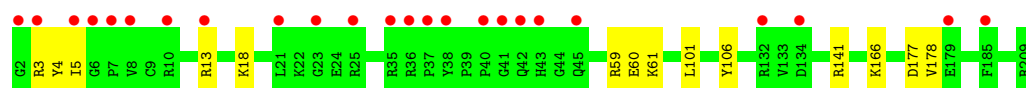
• Molecule 34: 30S ribosomal protein S3



• Molecule 34: 30S ribosomal protein S3

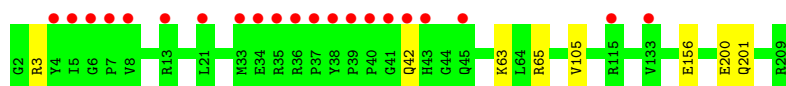


• Molecule 35: 30S ribosomal protein S4

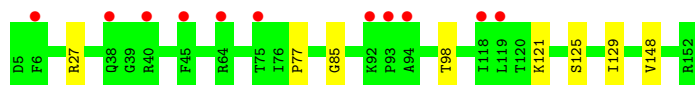


• Molecule 35: 30S ribosomal protein S4

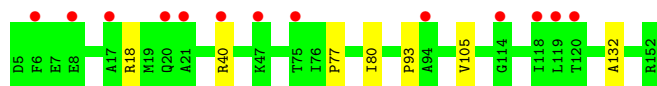




- Molecule 36: 30S ribosomal protein S5



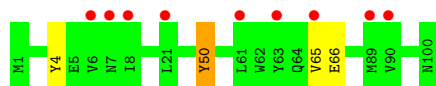
- Molecule 36: 30S ribosomal protein S5



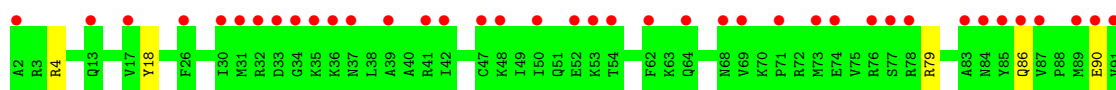
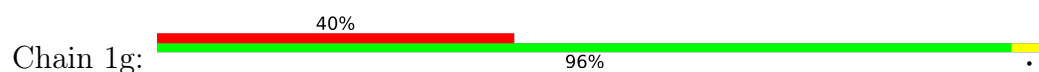
- Molecule 37: 30S ribosomal protein S6



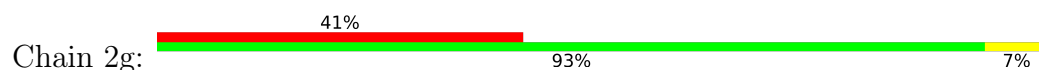
- Molecule 37: 30S ribosomal protein S6



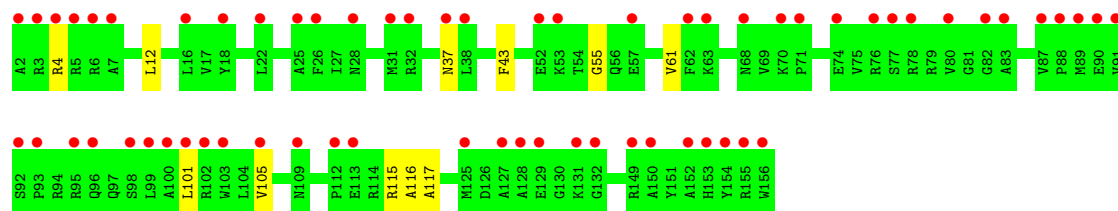
- Molecule 38: 30S ribosomal protein S7



- Molecule 38: 30S ribosomal protein S7



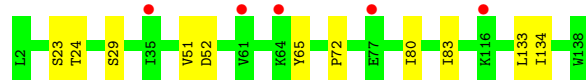
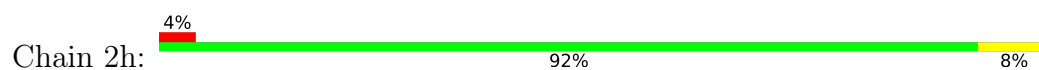




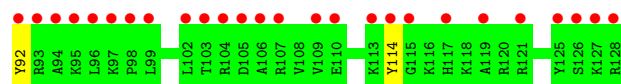
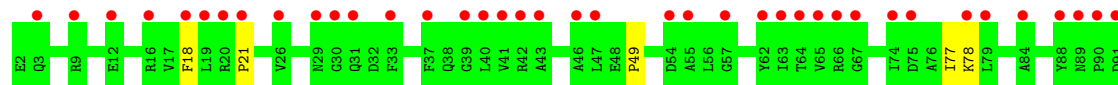
- Molecule 39: 30S ribosomal protein S8



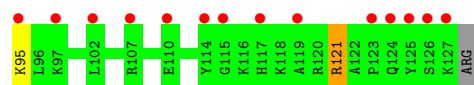
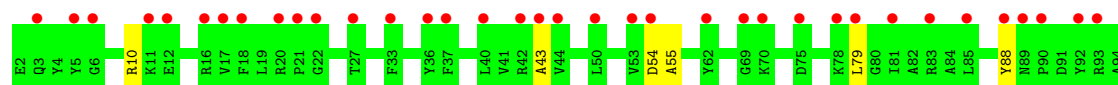
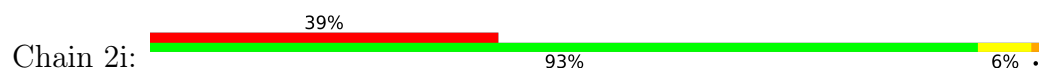
- Molecule 39: 30S ribosomal protein S8



- Molecule 40: 30S ribosomal protein S9

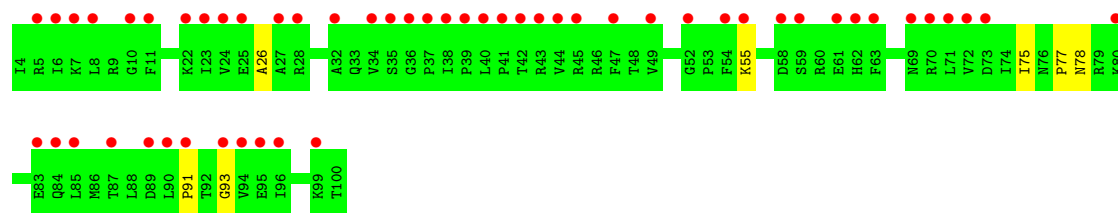


- Molecule 40: 30S ribosomal protein S9

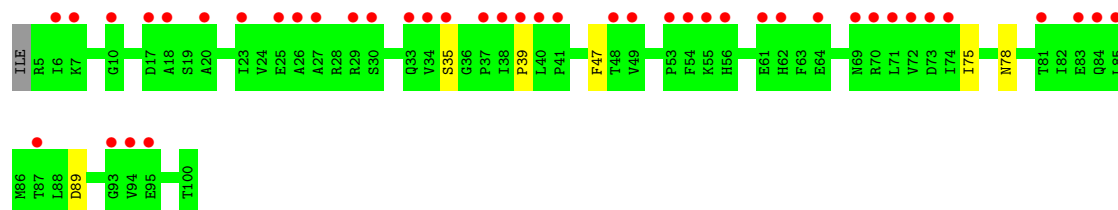
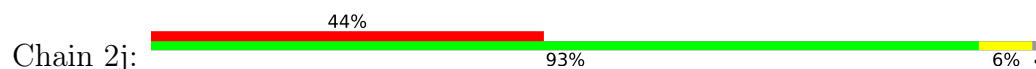


- Molecule 41: 30S ribosomal protein S10

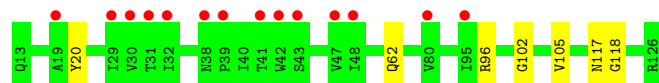




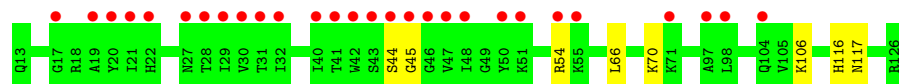
- Molecule 41: 30S ribosomal protein S10



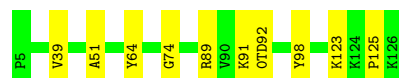
- Molecule 42: 30S ribosomal protein S11



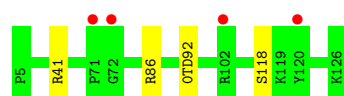
- Molecule 42: 30S ribosomal protein S11



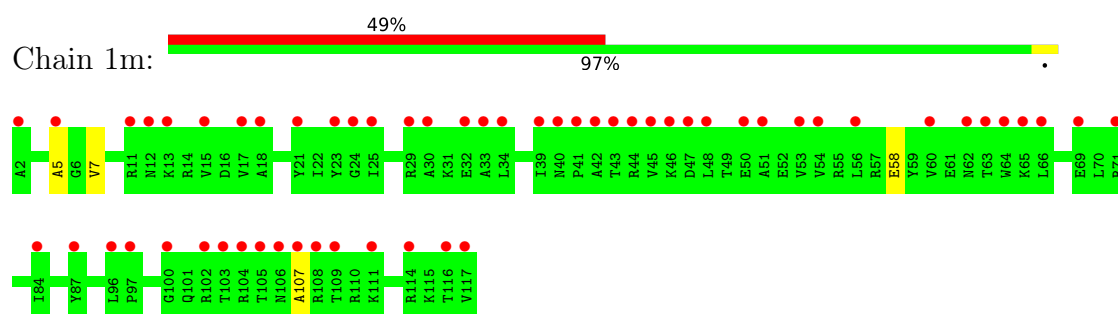
- Molecule 43: 30S ribosomal protein S12



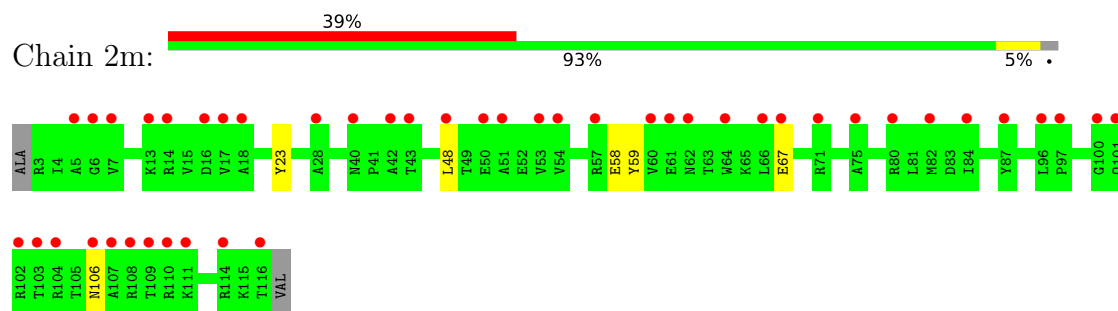
- Molecule 43: 30S ribosomal protein S12



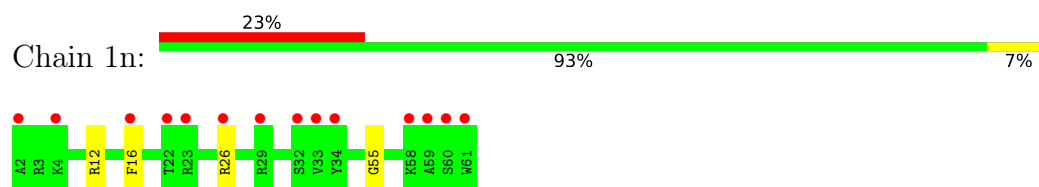
- Molecule 44: 30S ribosomal protein S13



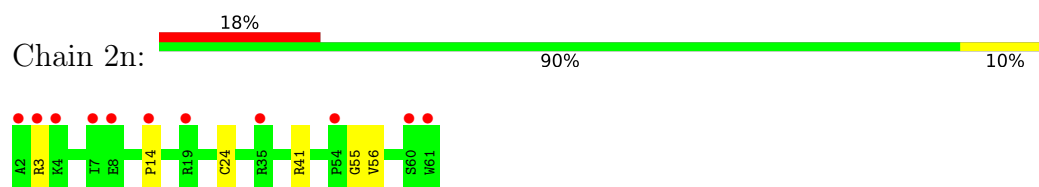
- Molecule 44: 30S ribosomal protein S13



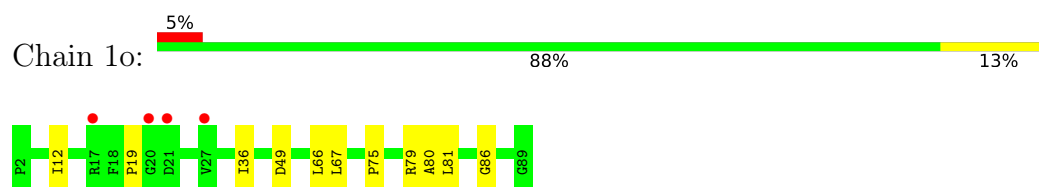
- Molecule 45: 30S ribosomal protein S14 type Z



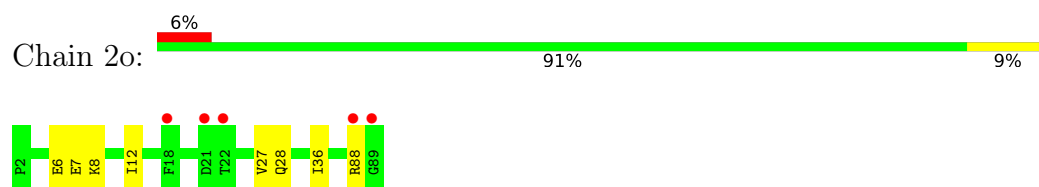
- Molecule 45: 30S ribosomal protein S14 type Z



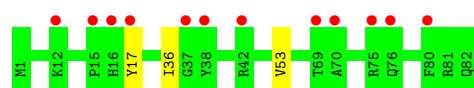
- Molecule 46: 30S ribosomal protein S15



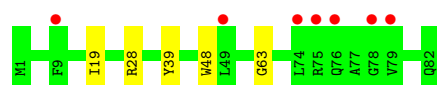
- Molecule 46: 30S ribosomal protein S15



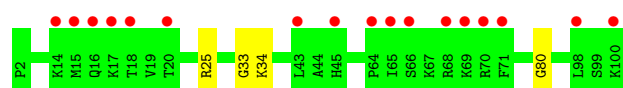
## ● Molecule 47: 30S ribosomal protein S16



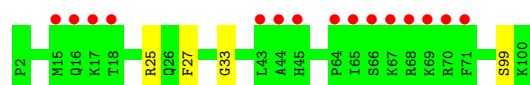
## ● Molecule 47: 30S ribosomal protein S16



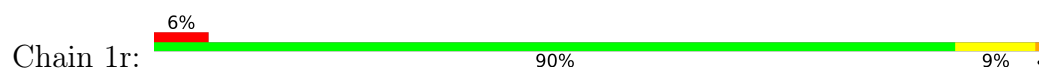
## ● Molecule 48: 30S ribosomal protein S17



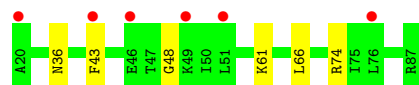
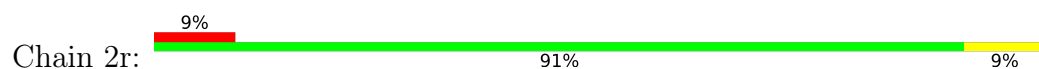
## ● Molecule 48: 30S ribosomal protein S17



## ● Molecule 49: 30S ribosomal protein S18

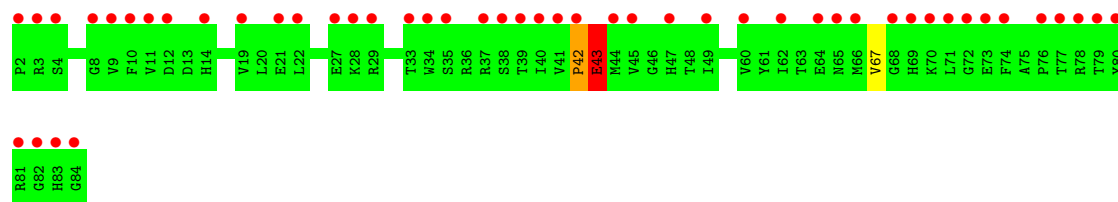


## ● Molecule 49: 30S ribosomal protein S18

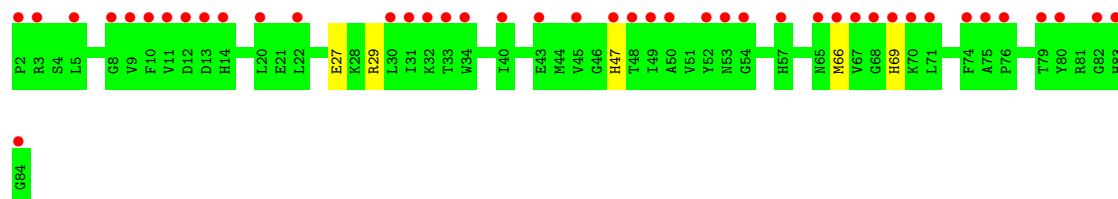


## ● Molecule 50: 30S ribosomal protein S19

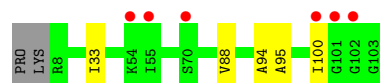




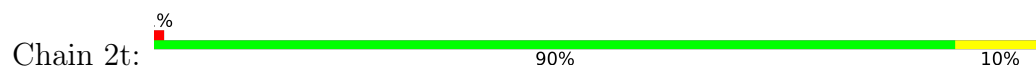
- Molecule 50: 30S ribosomal protein S19



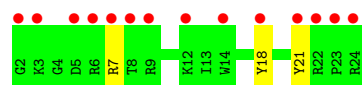
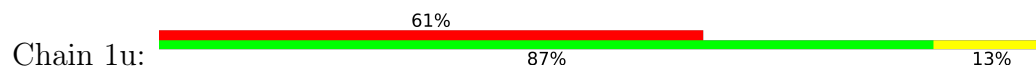
- Molecule 51: 30S ribosomal protein S20



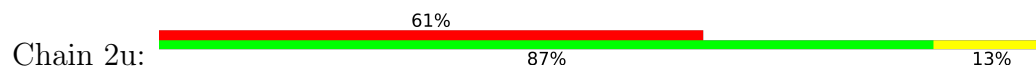
- Molecule 51: 30S ribosomal protein S20



- Molecule 52: 30S ribosomal protein Thx



- Molecule 52: 30S ribosomal protein Thx



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.04Å 449.52Å 624.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.92 – 3.14 49.92 – 3.14	Depositor EDS
% Data completeness (in resolution range)	97.8 (49.92-3.14) 97.9 (49.92-3.14)	Depositor EDS
$R_{merge}$	0.33	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.26 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, $R_{free}$	0.238 , 0.292 0.238 , 0.292	Depositor DCC
$R_{free}$ test set	49960 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	74.6	Xtriage
Anisotropy	0.421	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 97.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	290633	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	0.16	0/69029	0.72	4/107749 (0.0%)
1	2A	0.15	0/68903	0.71	5/107552 (0.0%)
2	1B	0.15	0/2876	0.71	0/4486
2	2B	0.14	0/2878	0.70	0/4490
3	1D	0.26	0/2181	0.50	1/2940 (0.0%)
3	2D	0.38	1/2186 (0.0%)	0.54	1/2944 (0.0%)
4	1E	0.26	0/1592	0.48	0/2149
4	2E	0.25	0/1592	0.49	0/2149
5	1F	0.25	0/1619	0.47	0/2193
5	2F	0.25	0/1615	0.44	0/2188
6	1G	0.24	0/1451	0.43	0/1961
6	2G	0.24	0/1449	0.44	0/1957
7	1H	0.24	0/1356	0.45	0/1834
7	2H	0.24	0/1350	0.46	0/1826
8	1I	0.24	0/1109	0.47	0/1512
8	2I	0.23	0/1095	0.42	0/1494
9	1N	0.24	0/1148	0.46	0/1547
9	2N	0.25	0/1144	0.46	0/1543
10	1O	0.25	0/943	0.47	0/1269
10	2O	0.27	0/943	0.48	0/1269
11	1P	0.25	0/1152	0.50	1/1533 (0.1%)
11	2P	0.24	0/1152	0.48	0/1533
12	1Q	0.25	0/1143	0.47	0/1527
12	2Q	0.25	0/1143	0.45	0/1527
13	1R	0.25	0/982	0.43	0/1312
13	2R	0.23	0/982	0.42	0/1312
14	1S	0.25	0/887	0.42	0/1180
14	2S	0.25	0/880	0.44	0/1172
15	1T	0.41	1/1105 (0.1%)	0.62	3/1477 (0.2%)
15	2T	0.31	0/1097	0.58	2/1468 (0.1%)
16	1U	0.25	0/977	0.49	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	2U	0.25	0/977	0.40	0/1301
17	1V	0.27	0/786	0.51	0/1053
17	2V	0.27	0/782	0.54	0/1049
18	1W	0.51	2/897 (0.2%)	1.02	5/1205 (0.4%)
18	2W	0.25	0/897	0.45	0/1205
19	1X	0.25	0/764	0.46	0/1025
19	2X	0.26	0/764	0.46	0/1025
20	1Y	0.25	0/823	0.46	0/1099
20	2Y	0.26	0/823	0.45	0/1100
21	1Z	0.25	0/1620	0.46	0/2200
21	2Z	0.27	0/1590	0.51	0/2162
22	10	0.24	0/616	0.45	0/821
22	20	0.25	0/616	0.48	0/821
23	11	0.25	0/761	0.46	0/1013
23	21	0.24	0/766	0.47	0/1018
24	12	0.22	0/590	0.39	0/781
24	22	0.23	0/594	0.43	0/785
25	13	0.23	0/474	0.42	0/635
25	23	0.23	0/469	0.41	0/630
26	14	0.30	0/559	0.56	0/754
26	24	0.26	0/549	0.48	0/741
27	15	0.26	0/473	0.46	0/639
27	25	0.26	0/469	0.42	0/635
28	16	0.24	0/460	0.48	0/613
28	26	0.24	0/456	0.46	0/608
29	17	0.22	0/426	0.45	0/561
29	27	0.23	0/426	0.47	0/561
30	18	0.25	0/525	0.44	0/691
30	28	0.25	0/525	0.45	0/691
31	19	0.35	0/310	0.51	0/407
31	29	0.24	0/310	0.46	0/407
32	1a	0.17	0/35795	0.74	1/55864 (0.0%)
32	2a	0.17	0/35890	0.73	1/56012 (0.0%)
33	1b	0.26	0/1876	0.53	2/2533 (0.1%)
33	2b	0.27	0/1860	0.47	0/2518
34	1c	0.25	0/1582	0.45	0/2137
34	2c	0.38	1/1566 (0.1%)	0.50	1/2119 (0.0%)
35	1d	0.27	0/1695	0.52	2/2274 (0.1%)
35	2d	0.25	0/1698	0.45	0/2277
36	1e	0.26	0/1149	0.47	0/1548
36	2e	0.25	0/1149	0.47	0/1548
37	1f	0.24	0/827	0.45	0/1120
37	2f	0.34	0/829	0.52	1/1123 (0.1%)



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	1g	0.23	0/1254	0.41	0/1683
38	2g	0.25	0/1248	0.43	0/1676
39	1h	0.25	0/1118	0.47	0/1506
39	2h	0.26	0/1108	0.45	0/1494
40	1i	0.27	0/1005	0.48	0/1351
40	2i	0.25	0/985	0.42	0/1329
41	1j	0.24	0/732	0.45	0/993
41	2j	0.24	0/723	0.45	0/984
42	1k	0.24	0/849	0.45	0/1150
42	2k	0.35	0/848	0.58	4/1149 (0.3%)
43	1l	0.25	0/937	0.50	0/1260
43	2l	0.24	0/937	0.48	0/1260
44	1m	0.23	0/924	0.46	0/1242
44	2m	0.23	0/905	0.44	0/1217
45	1n	0.26	0/501	0.47	0/664
45	2n	0.25	0/501	0.42	0/664
46	1o	0.23	0/739	0.43	0/985
46	2o	0.23	0/739	0.41	0/985
47	1p	0.24	0/697	0.46	0/939
47	2p	0.26	0/693	0.50	0/935
48	1q	0.24	0/836	0.44	0/1117
48	2q	0.24	0/836	0.44	0/1117
49	1r	0.36	0/560	0.55	1/746 (0.1%)
49	2r	0.26	0/560	0.47	0/746
50	1s	0.66	3/663 (0.5%)	0.89	4/895 (0.4%)
50	2s	0.25	0/660	0.51	0/893
51	1t	0.23	0/734	0.39	0/969
51	2t	0.25	0/736	0.40	0/976
52	1u	0.29	0/203	0.59	0/266
52	2u	0.26	0/203	0.51	0/266
All	All	0.20	8/308406 (0.0%)	0.66	39/461160 (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
3	2D	0	1
26	14	0	1
26	24	0	1
33	1b	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
42	2k	0	1
50	1s	0	2
All	All	0	7

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	1s	43	GLU	CB-CG	11.30	1.73	1.52
18	1W	11	ARG	CZ-NH1	10.31	1.46	1.33
34	2c	127	ARG	CG-CD	9.41	1.75	1.51
3	2D	275	LYS	CE-NZ	8.73	1.70	1.49
15	1T	74	ARG	CB-CG	7.28	1.72	1.52

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	1W	11	ARG	NE-CZ-NH2	-27.55	106.53	120.30
50	1s	43	GLU	OE1-CD-OE2	-14.46	105.94	123.30
15	1T	74	ARG	CG-CD-NE	9.00	130.71	111.80
15	2T	16	ARG	NE-CZ-NH1	-8.92	115.84	120.30
33	1b	209	ARG	NE-CZ-NH1	8.80	124.70	120.30

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	14	67	TYR	Peptide
33	1b	124	SER	Peptide
50	1s	42	PRO	Peptide
50	1s	43	GLU	Sidechain
3	2D	275	LYS	Peptide

## 5.2 Too-close contacts ⓘ

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

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/275 (99%)	222 (81%)	39 (14%)	12 (4%)	2	14
3	2D	273/275 (99%)	222 (81%)	46 (17%)	5 (2%)	8	33
4	1E	202/204 (99%)	170 (84%)	29 (14%)	3 (2%)	10	37
4	2E	202/204 (99%)	166 (82%)	31 (15%)	5 (2%)	5	25
5	1F	201/203 (99%)	173 (86%)	23 (11%)	5 (2%)	5	25
5	2F	201/203 (99%)	163 (81%)	33 (16%)	5 (2%)	5	25
6	1G	179/181 (99%)	137 (76%)	34 (19%)	8 (4%)	2	13
6	2G	179/181 (99%)	124 (69%)	43 (24%)	12 (7%)	1	6
7	1H	172/174 (99%)	144 (84%)	23 (13%)	5 (3%)	4	22
7	2H	171/174 (98%)	134 (78%)	27 (16%)	10 (6%)	1	9
8	1I	145/147 (99%)	119 (82%)	15 (10%)	11 (8%)	1	5
8	2I	144/147 (98%)	110 (76%)	24 (17%)	10 (7%)	1	6
9	1N	138/140 (99%)	118 (86%)	17 (12%)	3 (2%)	6	27
9	2N	138/140 (99%)	116 (84%)	15 (11%)	7 (5%)	2	11
10	1O	120/122 (98%)	98 (82%)	19 (16%)	3 (2%)	5	25
10	2O	120/122 (98%)	92 (77%)	22 (18%)	6 (5%)	2	12
11	1P	147/149 (99%)	129 (88%)	15 (10%)	3 (2%)	7	29
11	2P	147/149 (99%)	113 (77%)	28 (19%)	6 (4%)	3	15
12	1Q	139/141 (99%)	114 (82%)	17 (12%)	8 (6%)	1	9
12	2Q	139/141 (99%)	114 (82%)	22 (16%)	3 (2%)	6	27
13	1R	116/118 (98%)	95 (82%)	17 (15%)	4 (3%)	3	18
13	2R	116/118 (98%)	87 (75%)	20 (17%)	9 (8%)	1	5
14	1S	108/110 (98%)	85 (79%)	20 (18%)	3 (3%)	5	23
14	2S	108/110 (98%)	85 (79%)	20 (18%)	3 (3%)	5	23
15	1T	129/131 (98%)	99 (77%)	24 (19%)	6 (5%)	2	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	2T	129/131 (98%)	104 (81%)	23 (18%)	2 (2%)	9	35
16	1U	114/116 (98%)	99 (87%)	15 (13%)	0	100	100
16	2U	114/116 (98%)	89 (78%)	21 (18%)	4 (4%)	3	18
17	1V	99/101 (98%)	84 (85%)	12 (12%)	3 (3%)	4	21
17	2V	99/101 (98%)	80 (81%)	17 (17%)	2 (2%)	7	29
18	1W	110/112 (98%)	96 (87%)	11 (10%)	3 (3%)	5	23
18	2W	110/112 (98%)	80 (73%)	18 (16%)	12 (11%)	0	2
19	1X	93/95 (98%)	77 (83%)	13 (14%)	3 (3%)	4	20
19	2X	93/95 (98%)	80 (86%)	9 (10%)	4 (4%)	2	14
20	1Y	105/107 (98%)	95 (90%)	6 (6%)	4 (4%)	3	17
20	2Y	105/107 (98%)	85 (81%)	17 (16%)	3 (3%)	4	22
21	1Z	201/203 (99%)	161 (80%)	28 (14%)	12 (6%)	1	8
21	2Z	199/203 (98%)	148 (74%)	38 (19%)	13 (6%)	1	7
22	10	75/77 (97%)	61 (81%)	11 (15%)	3 (4%)	3	15
22	20	75/77 (97%)	58 (77%)	15 (20%)	2 (3%)	5	23
23	11	95/97 (98%)	80 (84%)	13 (14%)	2 (2%)	7	28
23	21	95/97 (98%)	84 (88%)	9 (10%)	2 (2%)	7	28
24	12	68/70 (97%)	55 (81%)	10 (15%)	3 (4%)	2	14
24	22	68/70 (97%)	51 (75%)	13 (19%)	4 (6%)	1	9
25	13	57/59 (97%)	51 (90%)	5 (9%)	1 (2%)	8	33
25	23	57/59 (97%)	47 (82%)	9 (16%)	1 (2%)	8	33
26	14	67/69 (97%)	48 (72%)	14 (21%)	5 (8%)	1	5
26	24	67/69 (97%)	45 (67%)	18 (27%)	4 (6%)	1	8
27	15	57/59 (97%)	49 (86%)	8 (14%)	0	100	100
27	25	57/59 (97%)	47 (82%)	10 (18%)	0	100	100
28	16	51/53 (96%)	41 (80%)	8 (16%)	2 (4%)	3	16
28	26	51/53 (96%)	44 (86%)	7 (14%)	0	100	100
29	17	46/48 (96%)	37 (80%)	7 (15%)	2 (4%)	2	14
29	27	46/48 (96%)	33 (72%)	13 (28%)	0	100	100
30	18	62/64 (97%)	57 (92%)	4 (6%)	1 (2%)	9	35
30	28	62/64 (97%)	54 (87%)	8 (13%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	19	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
31	29	35/37 (95%)	27 (77%)	7 (20%)	1 (3%)	4	22
33	1b	229/231 (99%)	164 (72%)	35 (15%)	30 (13%)	0	1
33	2b	229/231 (99%)	162 (71%)	48 (21%)	19 (8%)	1	4
34	1c	204/206 (99%)	161 (79%)	34 (17%)	9 (4%)	2	14
34	2c	204/206 (99%)	153 (75%)	40 (20%)	11 (5%)	2	10
35	1d	206/208 (99%)	157 (76%)	38 (18%)	11 (5%)	2	11
35	2d	206/208 (99%)	161 (78%)	39 (19%)	6 (3%)	4	22
36	1e	146/148 (99%)	121 (83%)	17 (12%)	8 (6%)	2	10
36	2e	146/148 (99%)	116 (80%)	24 (16%)	6 (4%)	3	15
37	1f	98/100 (98%)	75 (76%)	20 (20%)	3 (3%)	4	21
37	2f	98/100 (98%)	75 (76%)	21 (21%)	2 (2%)	7	29
38	1g	153/155 (99%)	120 (78%)	29 (19%)	4 (3%)	5	24
38	2g	153/155 (99%)	121 (79%)	23 (15%)	9 (6%)	1	9
39	1h	135/137 (98%)	104 (77%)	23 (17%)	8 (6%)	1	9
39	2h	135/137 (98%)	102 (76%)	23 (17%)	10 (7%)	1	5
40	1i	125/127 (98%)	92 (74%)	29 (23%)	4 (3%)	4	20
40	2i	124/127 (98%)	95 (77%)	21 (17%)	8 (6%)	1	7
41	1j	95/97 (98%)	72 (76%)	16 (17%)	7 (7%)	1	5
41	2j	94/97 (97%)	74 (79%)	15 (16%)	5 (5%)	2	11
42	1k	112/114 (98%)	86 (77%)	20 (18%)	6 (5%)	2	10
42	2k	112/114 (98%)	82 (73%)	24 (21%)	6 (5%)	2	10
43	1l	119/122 (98%)	92 (77%)	20 (17%)	7 (6%)	1	9
43	2l	119/122 (98%)	94 (79%)	22 (18%)	3 (2%)	5	25
44	1m	114/116 (98%)	89 (78%)	21 (18%)	4 (4%)	3	18
44	2m	112/116 (97%)	82 (73%)	24 (21%)	6 (5%)	2	10
45	1n	58/60 (97%)	45 (78%)	11 (19%)	2 (3%)	3	18
45	2n	58/60 (97%)	43 (74%)	9 (16%)	6 (10%)	0	2
46	1o	86/88 (98%)	57 (66%)	18 (21%)	11 (13%)	0	1
46	2o	86/88 (98%)	56 (65%)	22 (26%)	8 (9%)	0	3
47	1p	80/82 (98%)	66 (82%)	12 (15%)	2 (2%)	5	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	2p	80/82 (98%)	64 (80%)	12 (15%)	4 (5%)	2	12
48	1q	97/99 (98%)	75 (77%)	19 (20%)	3 (3%)	4	21
48	2q	97/99 (98%)	85 (88%)	9 (9%)	3 (3%)	4	21
49	1r	66/68 (97%)	49 (74%)	11 (17%)	6 (9%)	1	3
49	2r	66/68 (97%)	50 (76%)	11 (17%)	5 (8%)	1	5
50	1s	81/83 (98%)	58 (72%)	22 (27%)	1 (1%)	13	42
50	2s	81/83 (98%)	64 (79%)	12 (15%)	5 (6%)	1	8
51	1t	94/98 (96%)	76 (81%)	13 (14%)	5 (5%)	2	11
51	2t	96/98 (98%)	68 (71%)	18 (19%)	10 (10%)	0	2
52	1u	21/23 (91%)	19 (90%)	1 (5%)	1 (5%)	2	13
52	2u	21/23 (91%)	15 (71%)	4 (19%)	2 (10%)	0	3
All	All	11440/11648 (98%)	9049 (79%)	1872 (16%)	519 (4%)	2	13

5 of 519 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	1D	22	SER
3	1D	127	VAL
6	1G	49	ASP
6	1G	52	ILE
6	1G	110	ALA

### 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	214/217 (99%)	213 (100%)	1 (0%)	88	95
3	2D	215/217 (99%)	213 (99%)	2 (1%)	78	90
4	1E	164/165 (99%)	164 (100%)	0	100	100
4	2E	164/165 (99%)	163 (99%)	1 (1%)	86	94
5	1F	160/161 (99%)	157 (98%)	3 (2%)	57	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	2F	159/161 (99%)	154 (97%)	5 (3%)	40	69
6	1G	144/155 (93%)	144 (100%)	0	100	100
6	2G	142/155 (92%)	142 (100%)	0	100	100
7	1H	144/145 (99%)	143 (99%)	1 (1%)	84	93
7	2H	143/145 (99%)	142 (99%)	1 (1%)	84	93
8	1I	111/123 (90%)	111 (100%)	0	100	100
8	2I	109/123 (89%)	109 (100%)	0	100	100
9	1N	119/119 (100%)	118 (99%)	1 (1%)	81	92
9	2N	118/119 (99%)	116 (98%)	2 (2%)	60	82
10	1O	100/100 (100%)	99 (99%)	1 (1%)	76	89
10	2O	100/100 (100%)	99 (99%)	1 (1%)	76	89
11	1P	115/116 (99%)	115 (100%)	0	100	100
11	2P	115/116 (99%)	114 (99%)	1 (1%)	78	90
12	1Q	111/111 (100%)	108 (97%)	3 (3%)	44	72
12	2Q	111/111 (100%)	107 (96%)	4 (4%)	35	66
13	1R	101/101 (100%)	101 (100%)	0	100	100
13	2R	101/101 (100%)	101 (100%)	0	100	100
14	1S	87/87 (100%)	86 (99%)	1 (1%)	73	88
14	2S	85/87 (98%)	84 (99%)	1 (1%)	71	87
15	1T	115/115 (100%)	111 (96%)	4 (4%)	36	67
15	2T	113/115 (98%)	110 (97%)	3 (3%)	44	72
16	1U	93/93 (100%)	92 (99%)	1 (1%)	73	88
16	2U	93/93 (100%)	92 (99%)	1 (1%)	73	88
17	1V	81/82 (99%)	80 (99%)	1 (1%)	71	87
17	2V	80/82 (98%)	78 (98%)	2 (2%)	47	74
18	1W	90/91 (99%)	86 (96%)	4 (4%)	28	59
18	2W	90/91 (99%)	90 (100%)	0	100	100
19	1X	77/77 (100%)	76 (99%)	1 (1%)	69	86
19	2X	77/77 (100%)	75 (97%)	2 (3%)	46	73
20	1Y	86/88 (98%)	84 (98%)	2 (2%)	50	75
20	2Y	86/88 (98%)	85 (99%)	1 (1%)	71	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	1Z	169/176 (96%)	167 (99%)	2 (1%)	71	87
21	2Z	165/176 (94%)	161 (98%)	4 (2%)	49	75
22	10	61/62 (98%)	61 (100%)	0	100	100
22	20	61/62 (98%)	60 (98%)	1 (2%)	62	84
23	11	79/82 (96%)	79 (100%)	0	100	100
23	21	81/82 (99%)	81 (100%)	0	100	100
24	12	65/66 (98%)	65 (100%)	0	100	100
24	22	66/66 (100%)	65 (98%)	1 (2%)	65	84
25	13	51/51 (100%)	51 (100%)	0	100	100
25	23	50/51 (98%)	49 (98%)	1 (2%)	55	79
26	14	58/62 (94%)	56 (97%)	2 (3%)	37	67
26	24	54/62 (87%)	53 (98%)	1 (2%)	57	80
27	15	51/51 (100%)	49 (96%)	2 (4%)	32	63
27	25	50/51 (98%)	50 (100%)	0	100	100
28	16	51/51 (100%)	50 (98%)	1 (2%)	55	79
28	26	50/51 (98%)	50 (100%)	0	100	100
29	17	41/41 (100%)	41 (100%)	0	100	100
29	27	41/41 (100%)	40 (98%)	1 (2%)	49	75
30	18	54/54 (100%)	54 (100%)	0	100	100
30	28	54/54 (100%)	54 (100%)	0	100	100
31	19	34/34 (100%)	34 (100%)	0	100	100
31	29	34/34 (100%)	34 (100%)	0	100	100
33	1b	191/199 (96%)	189 (99%)	2 (1%)	76	89
33	2b	187/199 (94%)	185 (99%)	2 (1%)	73	88
34	1c	144/160 (90%)	142 (99%)	2 (1%)	67	85
34	2c	140/160 (88%)	139 (99%)	1 (1%)	84	93
35	1d	171/180 (95%)	170 (99%)	1 (1%)	86	94
35	2d	172/180 (96%)	170 (99%)	2 (1%)	71	87
36	1e	114/114 (100%)	114 (100%)	0	100	100
36	2e	114/114 (100%)	113 (99%)	1 (1%)	78	90
37	1f	85/90 (94%)	85 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	2f	85/90 (94%)	83 (98%)	2 (2%)	49	75
38	1g	120/126 (95%)	118 (98%)	2 (2%)	60	82
38	2g	119/126 (94%)	117 (98%)	2 (2%)	60	82
39	1h	116/118 (98%)	115 (99%)	1 (1%)	78	90
39	2h	114/118 (97%)	113 (99%)	1 (1%)	78	90
40	1i	91/98 (93%)	88 (97%)	3 (3%)	38	68
40	2i	88/98 (90%)	87 (99%)	1 (1%)	73	88
41	1j	68/87 (78%)	68 (100%)	0	100	100
41	2j	68/87 (78%)	67 (98%)	1 (2%)	65	84
42	1k	83/86 (96%)	82 (99%)	1 (1%)	71	87
42	2k	83/86 (96%)	83 (100%)	0	100	100
43	1l	96/102 (94%)	94 (98%)	2 (2%)	53	78
43	2l	96/102 (94%)	96 (100%)	0	100	100
44	1m	90/94 (96%)	90 (100%)	0	100	100
44	2m	87/94 (93%)	87 (100%)	0	100	100
45	1n	49/49 (100%)	47 (96%)	2 (4%)	30	61
45	2n	49/49 (100%)	49 (100%)	0	100	100
46	1o	78/79 (99%)	78 (100%)	0	100	100
46	2o	78/79 (99%)	78 (100%)	0	100	100
47	1p	69/71 (97%)	68 (99%)	1 (1%)	67	85
47	2p	68/71 (96%)	67 (98%)	1 (2%)	65	84
48	1q	94/94 (100%)	93 (99%)	1 (1%)	73	88
48	2q	94/94 (100%)	93 (99%)	1 (1%)	73	88
49	1r	59/59 (100%)	58 (98%)	1 (2%)	60	82
49	2r	59/59 (100%)	58 (98%)	1 (2%)	60	82
50	1s	68/72 (94%)	67 (98%)	1 (2%)	65	84
50	2s	67/72 (93%)	67 (100%)	0	100	100
51	1t	71/76 (93%)	71 (100%)	0	100	100
51	2t	70/76 (92%)	70 (100%)	0	100	100
52	1u	18/18 (100%)	16 (89%)	2 (11%)	6	23
52	2u	18/18 (100%)	17 (94%)	1 (6%)	21	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9364/9696 (97%)	9258 (99%)	106 (1%)	73 88

5 of 106 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
47	1p	17	TYR
5	2F	54	ARG
38	2g	37	ASN
49	1r	29	PHE
3	2D	9	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 128 such sidechains are listed below:

Mol	Chain	Res	Type
41	1j	56	HIS
3	2D	253	GLN
45	2n	49	HIS
43	1l	49	ASN
50	1s	83	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	485 (16%)	22 (0%)
1	2A	2857/2915 (98%)	519 (18%)	38 (1%)
2	1B	119/120 (99%)	13 (10%)	0
2	2B	119/120 (99%)	17 (14%)	0
32	1a	1494/2331 (64%)	278 (18%)	0
32	2a	1498/2331 (64%)	271 (18%)	0
All	All	8951/10732 (83%)	1583 (17%)	60 (0%)

5 of 1583 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	11	U
1	1A	12	A
1	1A	34	G
1	1A	38	C
1	1A	44	C

5 of 60 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2A	357	C
1	2A	902	C
1	2A	2193	U
1	2A	742	G
1	2A	1039	C

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	PSU	1A	1932	1	17,21,22	1.55	2 (11%)	20,30,33	3.07	7 (35%)
1	5MC	1A	1963	1	15,22,23	1.31	1 (6%)	19,32,35	1.33	3 (15%)
1	5MC	2A	1983	1	15,22,23	1.34	1 (6%)	19,32,35	1.33	3 (15%)
1	2MA	2A	2514	1,53	17,25,26	1.40	2 (11%)	19,37,40	2.12	3 (15%)
1	5MU	2A	1936	1	15,22,23	1.06	1 (6%)	16,32,35	1.87	2 (12%)
1	PSU	2A	2616	1	17,21,22	1.63	2 (11%)	20,30,33	3.23	6 (30%)
32	5MC	1a	1390	32	15,22,23	1.33	1 (6%)	19,32,35	1.29	3 (15%)
32	5MC	2a	1390	32	15,22,23	1.34	1 (6%)	19,32,35	1.31	3 (15%)
1	PSU	2A	1932	1	17,21,22	1.64	2 (11%)	20,30,33	3.15	6 (30%)
32	PSU	2a	500	32,53	17,21,22	1.62	3 (17%)	20,30,33	3.14	7 (35%)
43	0TD	1l	92	43	4,9,10	3.12	1 (25%)	3,11,13	12.88	1 (33%)
1	OMG	1A	2262	1,53	18,26,27	1.22	2 (11%)	20,38,41	2.26	6 (30%)
32	5MC	1a	1387	32	15,22,23	1.34	1 (6%)	19,32,35	1.32	3 (15%)
1	PSU	1A	1938	1	17,21,22	1.59	3 (17%)	20,30,33	3.06	6 (30%)
1	5MC	2A	1963	1	15,22,23	1.31	1 (6%)	19,32,35	1.30	3 (15%)
1	OMU	2A	2563	1,53	14,22,23	0.88	0	14,31,34	0.63	0
32	M2G	1a	944	32	20,27,28	1.39	3 (15%)	22,40,43	2.12	5 (22%)
1	5MU	2A	1960	1,53	15,22,23	1.08	1 (6%)	16,32,35	1.84	2 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
32	UR3	2a	1476	32	14,22,23	0.75	0	15,32,35	0.69	0
1	5MU	1A	1936	1	15,22,23	1.05	1 (6%)	16,32,35	1.86	2 (12%)
43	0TD	2l	92	43	4,9,10	3.06	1 (25%)	3,11,13	8.93	1 (33%)
32	5MC	2a	1387	32	15,22,23	1.28	1 (6%)	19,32,35	1.37	3 (15%)
32	MA6	1a	1497	32	19,26,27	1.01	1 (5%)	18,38,41	1.86	5 (27%)
32	M2G	2a	944	32	20,27,28	1.40	3 (15%)	22,40,43	2.10	5 (22%)
1	PSU	1A	2616	1	17,21,22	1.57	2 (11%)	20,30,33	3.13	6 (30%)
32	5MC	1a	1383	32	15,22,23	1.33	1 (6%)	19,32,35	1.31	3 (15%)
32	G7M	1a	511	32,53	20,26,27	2.84	4 (20%)	20,39,42	2.07	5 (25%)
1	2MA	1A	2514	1,53	17,25,26	1.41	2 (11%)	19,37,40	2.13	3 (15%)
1	OMC	1A	1941	1	15,22,23	0.63	0	17,31,34	1.32	2 (11%)
32	5MC	2a	1383	32	15,22,23	1.33	1 (6%)	19,32,35	1.33	3 (15%)
32	2MG	2a	1189	32	19,26,27	1.23	2 (10%)	21,38,41	2.18	7 (33%)
1	5MC	1A	1983	1	15,22,23	1.34	1 (6%)	19,32,35	1.32	3 (15%)
1	OMG	2A	2262	1,53	18,26,27	1.21	2 (11%)	20,38,41	2.17	6 (30%)
1	OMU	1A	2563	1,53	14,22,23	0.88	0	14,31,34	0.66	0
32	5MC	2a	945	32	15,22,23	1.32	1 (6%)	19,32,35	1.35	3 (15%)
32	PSU	1a	500	32,53	17,21,22	1.54	3 (17%)	20,30,33	3.06	6 (30%)
32	4OC	1a	1385	32	16,23,24	0.64	0	17,32,35	1.18	1 (5%)
32	MA6	2a	1497	32	19,26,27	1.00	1 (5%)	18,38,41	1.92	6 (33%)
32	G7M	2a	511	32,53	20,26,27	2.82	4 (20%)	20,39,42	2.11	6 (30%)
1	OMC	2A	1941	1	15,22,23	0.67	0	17,31,34	1.32	2 (11%)
32	MA6	1a	1496	32	19,26,27	0.99	1 (5%)	18,38,41	1.82	6 (33%)
32	UR3	1a	1476	32	14,22,23	0.74	0	15,32,35	0.70	0
32	MA6	2a	1496	32	19,26,27	0.99	1 (5%)	18,38,41	1.73	6 (33%)
1	5MU	1A	1960	1	15,22,23	1.11	2 (13%)	16,32,35	1.84	2 (12%)
1	PSU	2A	1938	1	17,21,22	1.64	2 (11%)	20,30,33	3.22	6 (30%)
32	5MC	1a	945	32	15,22,23	1.32	1 (6%)	19,32,35	1.33	3 (15%)
32	4OC	2a	1385	32	16,23,24	0.62	0	17,32,35	1.15	1 (5%)
32	2MG	1a	1189	32,53	19,26,27	1.27	2 (10%)	21,38,41	2.26	7 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	1A	1932	1	-	0/7/25/26	0/2/2/2
1	5MC	1A	1963	1	-	0/5/25/26	0/2/2/2
1	5MC	2A	1983	1	-	1/5/25/26	0/2/2/2
1	2MA	2A	2514	1,53	-	2/3/25/26	0/3/3/3
1	5MU	2A	1936	1	-	0/5/25/26	0/2/2/2
1	PSU	2A	2616	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	1390	32	-	0/5/25/26	0/2/2/2
32	5MC	2a	1390	32	-	0/5/25/26	0/2/2/2
1	PSU	2A	1932	1	-	0/7/25/26	0/2/2/2
32	PSU	2a	500	32,53	-	2/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	1/3/12/14	-
1	OMG	1A	2262	1,53	-	0/5/27/28	0/3/3/3
32	5MC	1a	1387	32	-	0/5/25/26	0/2/2/2
1	PSU	1A	1938	1	-	1/7/25/26	0/2/2/2
1	5MC	2A	1963	1	-	2/5/25/26	0/2/2/2
1	OMU	2A	2563	1,53	-	0/7/27/28	0/2/2/2
32	M2G	1a	944	32	-	0/7/29/30	0/3/3/3
1	5MU	2A	1960	1,53	-	0/5/25/26	0/2/2/2
32	UR3	2a	1476	32	-	2/5/25/26	0/2/2/2
1	5MU	1A	1936	1	-	0/5/25/26	0/2/2/2
43	0TD	2l	92	43	-	2/3/12/14	-
32	5MC	2a	1387	32	-	0/5/25/26	0/2/2/2
32	MA6	1a	1497	32	-	3/7/29/30	0/3/3/3
32	M2G	2a	944	32	-	4/7/29/30	0/3/3/3
1	PSU	1A	2616	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	1383	32	-	2/5/25/26	0/2/2/2
32	G7M	1a	511	32,53	-	2/3/25/26	0/3/3/3
1	2MA	1A	2514	1,53	-	1/3/25/26	0/3/3/3
1	OMC	1A	1941	1	-	1/7/27/28	0/2/2/2
32	5MC	2a	1383	32	-	2/5/25/26	0/2/2/2
32	2MG	2a	1189	32	-	0/5/27/28	0/3/3/3
1	5MC	1A	1983	1	-	0/5/25/26	0/2/2/2
1	OMG	2A	2262	1,53	-	0/5/27/28	0/3/3/3
1	OMU	1A	2563	1,53	-	1/7/27/28	0/2/2/2
32	5MC	2a	945	32	-	0/5/25/26	0/2/2/2
32	PSU	1a	500	32,53	-	0/7/25/26	0/2/2/2
32	4OC	1a	1385	32	-	0/9/29/30	0/2/2/2
32	MA6	2a	1497	32	-	6/7/29/30	0/3/3/3
32	G7M	2a	511	32,53	-	2/3/25/26	0/3/3/3
1	OMC	2A	1941	1	-	2/7/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	MA6	1a	1496	32	-	1/7/29/30	0/3/3/3
32	UR3	1a	1476	32	-	2/5/25/26	0/2/2/2
32	MA6	2a	1496	32	-	3/7/29/30	0/3/3/3
1	5MU	1A	1960	1	-	2/5/25/26	0/2/2/2
1	PSU	2A	1938	1	-	1/7/25/26	0/2/2/2
32	5MC	1a	945	32	-	0/5/25/26	0/2/2/2
32	4OC	2a	1385	32	-	4/9/29/30	0/2/2/2
32	2MG	1a	1189	32,53	-	0/5/27/28	0/3/3/3

The worst 5 of 68 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1a	511	G7M	C8-N9	7.38	1.46	1.33
32	2a	511	G7M	C8-N9	7.34	1.46	1.33
32	1a	511	G7M	C8-N7	7.27	1.46	1.33
32	2a	511	G7M	C8-N7	7.13	1.46	1.33
32	2a	511	G7M	C5-C4	6.02	1.47	1.39

The worst 5 of 178 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1l	92	0TD	CSB-SB-CB	-22.24	58.11	101.85
43	2l	92	0TD	CSB-SB-CB	-15.40	71.57	101.85
32	2a	500	PSU	N1-C2-N3	-8.58	121.61	128.43
32	1a	500	PSU	N1-C2-N3	-8.41	121.75	128.43
1	1A	1932	PSU	N1-C2-N3	-8.28	121.84	128.43

There are no chirality outliers.

5 of 52 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	2A	1983	5MC	O4'-C1'-N1-C6
1	2A	1963	5MC	O4'-C4'-C5'-O5'
32	2a	1476	UR3	O4'-C1'-N1-C6
32	2a	1476	UR3	C2'-C1'-N1-C6
43	2l	92	0TD	CG-CB-SB-CSB

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 1955 ligands modelled in this entry, 1942 are monoatomic - leaving 13 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
55	MPD	18	104	-	7,7,7	0.28	0	9,10,10	0.25	0
54	ARG	1A	3799	-	7,11,11	0.26	0	6,13,13	0.25	0
55	MPD	1T	8004	-	7,7,7	0.28	0	9,10,10	0.29	0
55	MPD	1a	1900	-	7,7,7	0.30	0	9,10,10	0.24	0
56	FSD	2A	3553	-	40,47,47	1.52	6 (15%)	49,69,69	2.17	15 (30%)
58	SF4	2d	501	35	0,12,12	0.00	-	-	-	-
55	MPD	2B	210	-	7,7,7	0.26	0	9,10,10	0.20	0
56	FSD	1A	3801	-	40,47,47	1.27	5 (12%)	49,69,69	1.41	5 (10%)
55	MPD	2A	3552	-	7,7,7	0.27	0	9,10,10	0.24	0
54	ARG	1B	223	53	7,11,11	0.26	0	6,13,13	0.30	0
55	MPD	1A	3800	53	7,7,7	0.27	0	9,10,10	0.24	0
58	SF4	1d	501	35	0,12,12	0.00	-	-	-	-
55	MPD	2A	3551	-	7,7,7	0.27	0	9,10,10	0.21	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	MPD	18	104	-	-	2/5/5/5	-
54	ARG	1A	3799	-	-	0/7/11/11	-
55	MPD	1T	8004	-	-	5/5/5/5	-
55	MPD	1a	1900	-	-	2/5/5/5	-
56	FSD	2A	3553	-	-	14/27/66/66	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	SF4	2d	501	35	-	-	0/6/5/5
55	MPD	2B	210	-	-	2/5/5/5	-
56	FSD	1A	3801	-	-	4/27/66/66	0/4/4/4
55	MPD	2A	3552	-	-	4/5/5/5	-
54	ARG	1B	223	53	-	0/7/11/11	-
55	MPD	1A	3800	53	-	2/5/5/5	-
58	SF4	1d	501	35	-	-	0/6/5/5
55	MPD	2A	3551	-	-	4/5/5/5	-

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	2A	3553	FSD	OAY-CBM	-3.91	1.37	1.42
56	2A	3553	FSD	CBF-NAV	-3.74	1.26	1.34
56	2A	3553	FSD	CBO-NBP	3.40	1.57	1.48
56	1A	3801	FSD	CBO-NBP	3.04	1.56	1.48
56	2A	3553	FSD	CBF-NAX	-2.79	1.34	1.40

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	2A	3553	FSD	OAH-CBC-CBR	-7.11	112.35	120.38
56	1A	3801	FSD	OAY-CBM-NBQ	6.76	113.40	105.92
56	2A	3553	FSD	CAC-NBP-CBO	4.69	124.69	113.59
56	2A	3553	FSD	CBN-CBJ-CBK	-4.34	100.96	110.00
56	2A	3553	FSD	OBA-CBN-CBJ	3.92	118.25	108.10

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	1a	1900	MPD	C2-C3-C4-O4
56	2A	3553	FSD	CAQ-CBF-NAX-CBB
56	2A	3553	FSD	NAV-CBF-NAX-CBB
56	2A	3553	FSD	CBI-CBO-NBP-CAC
56	2A	3553	FSD	CBK-CBO-NBP-CAC

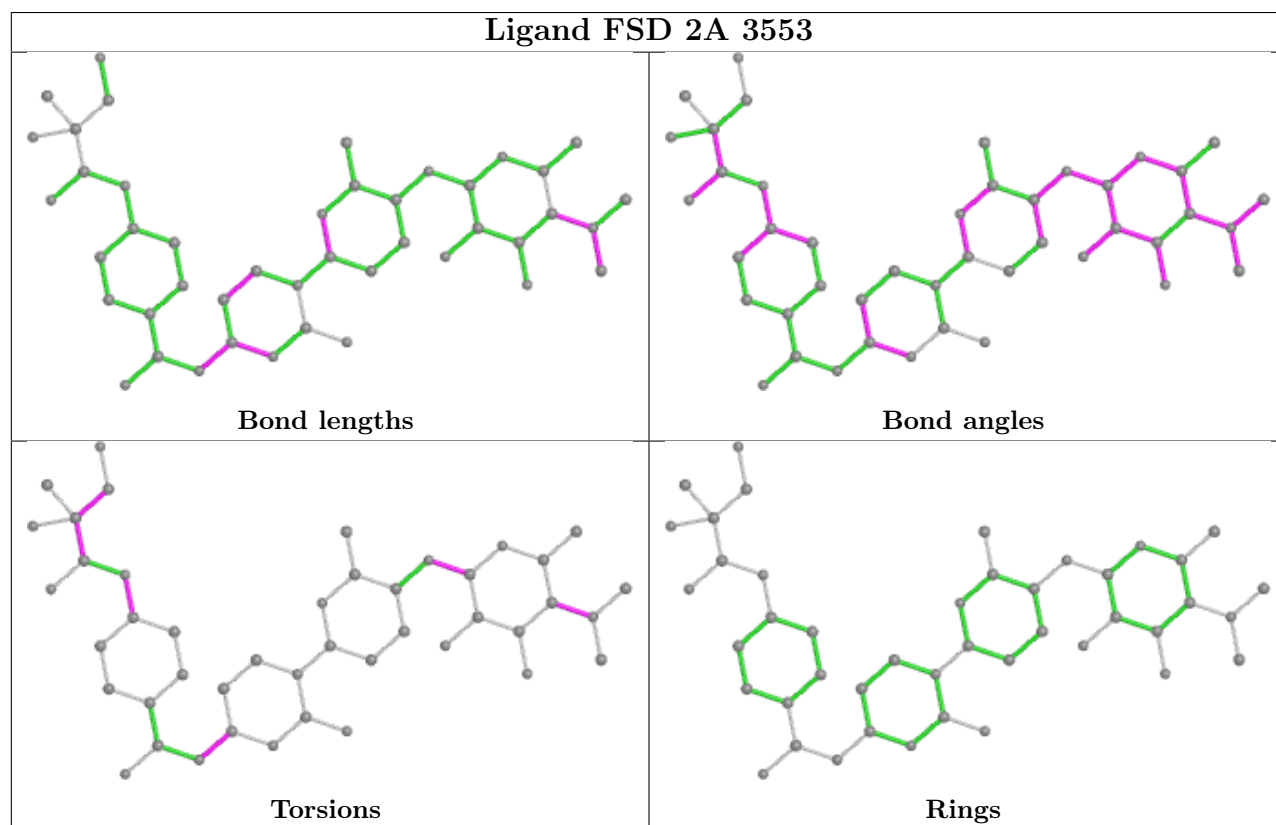
There are no ring outliers.

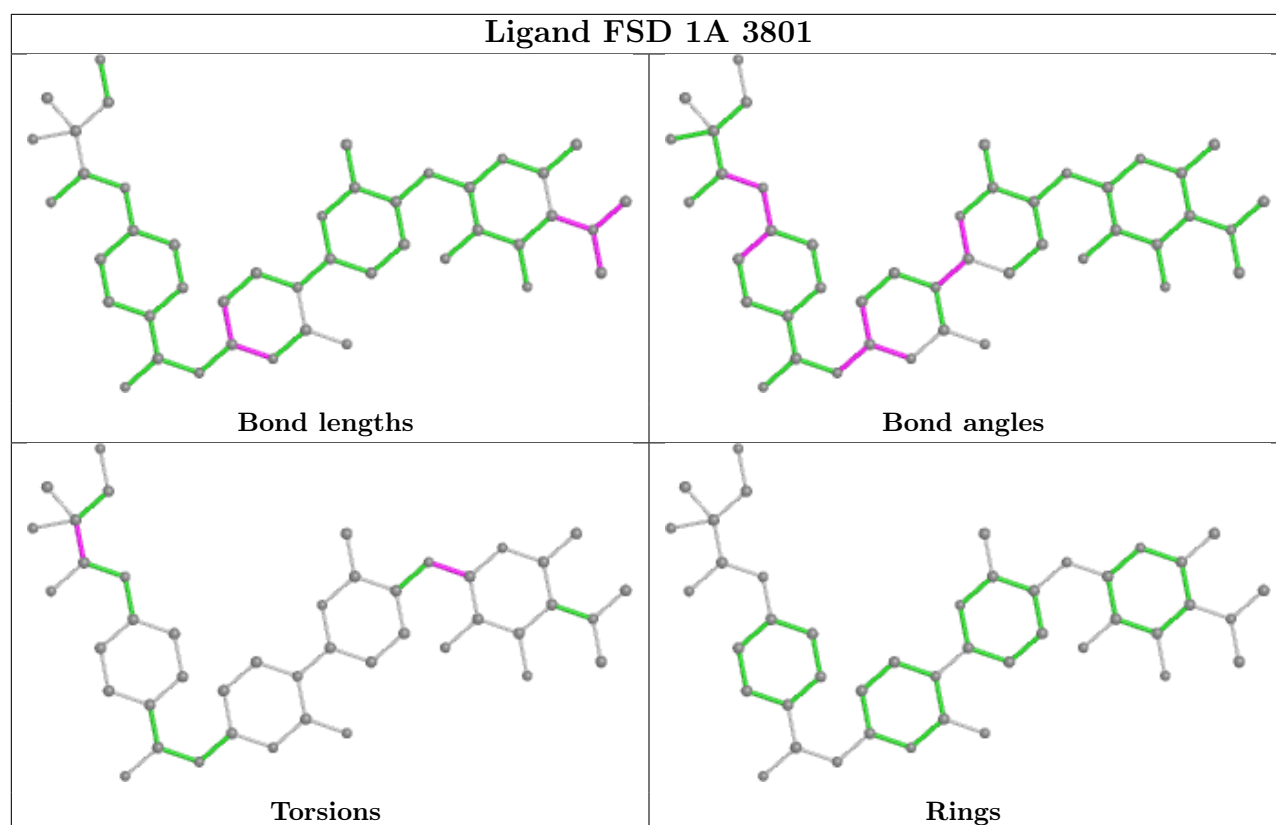
No monomer is involved in short contacts.

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	1A	2861/2915 (98%)	0.57	182 (6%) 19 8	26, 55, 217, 326	0
1	2A	2856/2915 (97%)	0.65	239 (8%) 11 4	56, 89, 195, 358	0
2	1B	120/120 (100%)	0.16	1 (0%) 86 74	35, 70, 93, 122	0
2	2B	120/120 (100%)	0.75	10 (8%) 11 4	83, 134, 160, 179	0
3	1D	275/275 (100%)	-0.12	0 100 100	29, 54, 74, 105	0
3	2D	275/275 (100%)	0.02	3 (1%) 80 66	53, 78, 100, 112	0
4	1E	204/204 (100%)	-0.10	2 (0%) 82 70	26, 54, 75, 100	0
4	2E	204/204 (100%)	0.24	10 (4%) 29 14	60, 96, 131, 142	0
5	1F	203/203 (100%)	-0.02	2 (0%) 82 70	26, 59, 96, 165	0
5	2F	203/203 (100%)	0.19	6 (2%) 50 29	57, 91, 124, 143	0
6	1G	181/181 (100%)	0.65	29 (16%) 1 1	67, 120, 158, 180	0
6	2G	181/181 (100%)	1.55	54 (29%) 0 0	124, 175, 205, 217	0
7	1H	174/174 (100%)	-0.25	0 100 100	39, 69, 88, 101	0
7	2H	173/174 (99%)	0.89	31 (17%) 1 0	104, 144, 172, 178	0
8	1I	147/147 (100%)	0.30	16 (10%) 5 2	60, 113, 135, 160	0
8	2I	146/147 (99%)	0.49	20 (13%) 3 1	83, 132, 152, 162	0
9	1N	140/140 (100%)	-0.21	0 100 100	33, 50, 73, 88	0
9	2N	140/140 (100%)	-0.06	2 (1%) 75 59	76, 106, 125, 143	0
10	1O	122/122 (100%)	-0.21	0 100 100	41, 58, 77, 89	0
10	2O	122/122 (100%)	-0.05	1 (0%) 86 74	62, 91, 108, 121	0
11	1P	149/149 (100%)	0.03	0 100 100	27, 64, 95, 123	0
11	2P	149/149 (100%)	0.28	9 (6%) 21 10	62, 97, 129, 145	0
12	1Q	141/141 (100%)	-0.11	0 100 100	35, 53, 72, 101	0
12	2Q	141/141 (100%)	0.08	2 (1%) 75 59	75, 102, 124, 140	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	1R	118/118 (100%)	-0.10	0 100 100	33, 50, 69, 81	0
13	2R	118/118 (100%)	0.04	0 100 100	66, 84, 100, 114	0
14	1S	110/110 (100%)	0.25	3 (2%) 54 32	41, 65, 91, 110	0
14	2S	110/110 (100%)	0.98	16 (14%) 2 1	96, 125, 147, 153	0
15	1T	131/131 (100%)	-0.09	0 100 100	45, 63, 96, 118	0
15	2T	131/131 (100%)	-0.08	3 (2%) 60 40	76, 100, 124, 141	0
16	1U	116/116 (100%)	-0.04	0 100 100	27, 45, 63, 90	0
16	2U	116/116 (100%)	0.23	4 (3%) 45 24	61, 99, 125, 131	0
17	1V	101/101 (100%)	-0.27	0 100 100	32, 51, 76, 97	0
17	2V	101/101 (100%)	0.40	5 (4%) 28 13	61, 104, 130, 153	0
18	1W	112/112 (100%)	-0.01	1 (0%) 84 72	21, 42, 70, 104	0
18	2W	112/112 (100%)	-0.09	1 (0%) 84 72	51, 70, 96, 121	0
19	1X	95/95 (100%)	-0.28	0 100 100	33, 53, 76, 97	0
19	2X	95/95 (100%)	-0.10	1 (1%) 80 66	60, 79, 104, 132	0
20	1Y	107/107 (100%)	-0.19	2 (1%) 66 48	47, 65, 95, 117	0
20	2Y	107/107 (100%)	0.43	10 (9%) 8 3	69, 100, 131, 145	0
21	1Z	203/203 (100%)	-0.20	1 (0%) 91 83	47, 72, 102, 115	0
21	2Z	201/203 (99%)	0.54	22 (10%) 5 2	92, 124, 151, 174	0
22	10	77/77 (100%)	-0.05	1 (1%) 77 61	34, 51, 73, 121	0
22	20	77/77 (100%)	0.34	3 (3%) 39 20	71, 92, 111, 132	0
23	11	97/97 (100%)	-0.04	0 100 100	39, 60, 88, 98	0
23	21	97/97 (100%)	0.04	2 (2%) 63 44	58, 85, 116, 127	0
24	12	70/70 (100%)	-0.08	1 (1%) 75 59	40, 63, 82, 100	0
24	22	70/70 (100%)	-0.08	1 (1%) 75 59	72, 90, 112, 129	0
25	13	59/59 (100%)	-0.29	0 100 100	31, 48, 71, 105	0
25	23	59/59 (100%)	0.24	4 (6%) 17 7	71, 98, 124, 134	0
26	14	69/69 (100%)	1.55	21 (30%) 0 0	110, 160, 235, 240	0
26	24	69/69 (100%)	2.28	32 (46%) 0 0	157, 208, 229, 241	0
27	15	59/59 (100%)	-0.16	0 100 100	29, 46, 72, 76	0
27	25	59/59 (100%)	0.15	1 (1%) 70 51	64, 82, 112, 122	0
28	16	53/53 (100%)	-0.01	0 100 100	43, 57, 78, 94	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
28	26	53/53 (100%)	0.42	3 (5%)	23 11	74, 87, 104, 113	0
29	17	48/48 (100%)	0.07	1 (2%)	63 44	30, 44, 79, 97	0
29	27	48/48 (100%)	0.07	0	100 100	52, 66, 99, 115	0
30	18	64/64 (100%)	0.05	0	100 100	34, 51, 61, 66	0
30	28	64/64 (100%)	0.16	0	100 100	63, 81, 97, 112	0
31	19	37/37 (100%)	0.23	0	100 100	41, 53, 72, 92	0
31	29	37/37 (100%)	0.68	3 (8%)	12 5	84, 108, 138, 148	0
32	1a	1488/2331 (63%)	1.21	330 (22%)	0 0	55, 122, 256, 317	0
32	2a	1492/2331 (64%)	1.26	350 (23%)	0 0	75, 132, 247, 372	0
33	1b	231/231 (100%)	0.53	30 (12%)	3 1	112, 142, 168, 180	0
33	2b	231/231 (100%)	0.95	42 (18%)	1 0	127, 163, 187, 203	0
34	1c	206/206 (100%)	1.71	68 (33%)	0 0	139, 173, 194, 208	0
34	2c	206/206 (100%)	1.54	67 (32%)	0 0	139, 173, 189, 203	0
35	1d	208/208 (100%)	0.42	24 (11%)	4 2	100, 129, 150, 161	0
35	2d	208/208 (100%)	0.36	21 (10%)	7 2	100, 126, 148, 158	0
36	1e	148/148 (100%)	0.31	11 (7%)	14 6	81, 113, 139, 161	0
36	2e	148/148 (100%)	0.48	13 (8%)	10 4	102, 121, 140, 158	0
37	1f	100/100 (100%)	0.08	5 (5%)	28 13	81, 108, 126, 136	0
37	2f	100/100 (100%)	0.26	9 (9%)	9 4	106, 127, 142, 157	0
38	1g	155/155 (100%)	1.89	62 (40%)	0 0	150, 188, 208, 223	0
38	2g	155/155 (100%)	1.89	63 (40%)	0 0	153, 183, 197, 210	0
39	1h	137/137 (100%)	-0.00	1 (0%)	87 77	85, 107, 123, 141	0
39	2h	137/137 (100%)	0.12	5 (3%)	42 22	100, 125, 144, 157	0
40	1i	127/127 (100%)	2.18	65 (51%)	0 0	157, 206, 220, 229	0
40	2i	126/127 (99%)	2.04	50 (39%)	0 0	167, 203, 221, 233	0
41	1j	97/97 (100%)	2.66	53 (54%)	0 0	173, 205, 221, 230	0
41	2j	96/97 (98%)	2.19	43 (44%)	0 0	156, 193, 215, 222	0
42	1k	114/114 (100%)	0.60	14 (12%)	4 1	69, 107, 127, 144	0
42	2k	114/114 (100%)	1.05	28 (24%)	0 0	98, 129, 145, 156	0
43	1l	121/122 (99%)	0.08	0	100 100	62, 102, 120, 133	0
43	2l	121/122 (99%)	0.17	4 (3%)	46 25	83, 111, 125, 136	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	1m	116/116 (100%)	2.38	57 (49%) 0 0	187, 228, 248, 257	0
44	2m	114/116 (98%)	2.27	45 (39%) 0 0	188, 217, 227, 233	0
45	1n	60/60 (100%)	1.46	14 (23%) 0 0	165, 192, 219, 228	0
45	2n	60/60 (100%)	1.03	11 (18%) 1 0	166, 190, 213, 220	0
46	1o	88/88 (100%)	0.08	4 (4%) 33 16	67, 101, 121, 128	0
46	2o	88/88 (100%)	0.18	5 (5%) 23 11	83, 118, 138, 152	0
47	1p	82/82 (100%)	0.69	12 (14%) 2 1	103, 125, 150, 176	0
47	2p	82/82 (100%)	0.57	7 (8%) 10 4	101, 123, 145, 160	0
48	1q	99/99 (100%)	0.56	17 (17%) 1 1	74, 98, 112, 128	0
48	2q	99/99 (100%)	0.59	15 (15%) 2 1	93, 112, 126, 131	0
49	1r	68/68 (100%)	0.38	4 (5%) 22 10	78, 102, 127, 142	0
49	2r	68/68 (100%)	0.75	6 (8%) 10 4	108, 127, 150, 158	0
50	1s	83/83 (100%)	2.87	49 (59%) 0 0	175, 227, 240, 242	0
50	2s	83/83 (100%)	2.58	43 (51%) 0 0	157, 222, 233, 240	0
51	1t	96/98 (97%)	0.26	6 (6%) 20 9	80, 111, 125, 133	0
51	2t	98/98 (100%)	0.14	1 (1%) 82 70	98, 118, 144, 152	0
52	1u	23/23 (100%)	2.85	14 (60%) 0 0	203, 216, 226, 235	0
52	2u	23/23 (100%)	3.01	14 (60%) 0 0	195, 210, 221, 226	0
All	All	20573/22380 (91%)	0.64	2443 (11%) 4 2	21, 100, 220, 372	0

The worst 5 of 2443 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
41	1j	71	LEU	22.4
32	2a	1019	G	15.4
32	1a	1019	G	14.9
44	2m	6	GLY	13.9
6	2G	41	GLN	13.5

## 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
32	5MC	1a	945	21/22	0.69	0.37	167,190,209,211	0
32	2MG	1a	1189	24/25	0.77	0.47	211,226,238,245	0
32	5MC	2a	945	21/22	0.77	0.24	148,172,188,202	0
32	M2G	1a	944	25/26	0.78	0.29	174,190,199,215	0
32	2MG	2a	1189	24/25	0.80	0.35	180,204,208,221	0
1	OMC	1A	1941	21/22	0.81	0.40	95,110,120,128	0
1	PSU	2A	1938	20/21	0.83	0.34	135,154,172,183	0
32	M2G	2a	944	25/26	0.84	0.29	149,173,196,215	0
32	5MC	2a	1390	21/22	0.84	0.33	111,129,139,149	0
32	G7M	2a	511	24/25	0.84	0.28	94,123,134,141	0
32	PSU	1a	500	20/21	0.85	0.25	94,120,144,149	0
1	OMC	2A	1941	21/22	0.86	0.42	121,133,143,165	0
32	PSU	2a	500	20/21	0.86	0.32	120,144,167,167	0
32	4OC	2a	1385	22/23	0.88	0.29	109,124,128,131	0
32	5MC	2a	1387	21/22	0.88	0.19	102,127,139,146	0
1	5MU	1A	1936	21/22	0.89	0.34	121,142,154,157	0
1	PSU	2A	1932	20/21	0.89	0.33	119,134,142,160	0
32	MA6	2a	1496	24/25	0.89	0.25	108,121,129,133	0
43	0TD	2l	92	10/11	0.90	0.18	103,114,130,148	0
1	PSU	1A	1938	20/21	0.90	0.37	110,132,143,150	0
32	MA6	2a	1497	24/25	0.90	0.27	98,115,131,143	0
43	0TD	1l	92	10/11	0.91	0.23	94,117,125,174	0
1	5MU	2A	1936	21/22	0.91	0.33	138,161,170,174	0
1	OMG	2A	2262	24/25	0.91	0.26	68,87,96,102	0
32	5MC	1a	1390	21/22	0.92	0.24	77,91,105,108	0
1	5MC	2A	1983	21/22	0.92	0.18	70,80,88,108	0
32	5MC	2a	1383	21/22	0.92	0.19	105,128,143,145	0
1	PSU	1A	1932	20/21	0.93	0.46	102,112,120,121	0
32	5MC	1a	1383	21/22	0.93	0.17	87,107,122,125	0
32	5MC	1a	1387	21/22	0.93	0.20	60,85,98,106	0
32	UR3	2a	1476	21/22	0.93	0.20	78,115,129,130	0
32	MA6	1a	1496	24/25	0.94	0.21	54,73,87,88	0
1	PSU	2A	2616	20/21	0.94	0.19	54,71,80,96	0
32	G7M	1a	511	24/25	0.94	0.19	89,108,122,128	0
32	MA6	1a	1497	24/25	0.94	0.21	63,81,94,96	0
1	5MC	2A	1963	21/22	0.94	0.16	79,95,105,115	0
1	OMG	1A	2262	24/25	0.95	0.22	31,43,50,70	0
32	UR3	1a	1476	21/22	0.95	0.17	80,91,105,107	0
32	4OC	1a	1385	22/23	0.95	0.23	72,92,108,122	0
1	5MC	1A	1983	21/22	0.95	0.20	26,60,76,94	0
1	2MA	2A	2514	23/24	0.95	0.24	49,61,71,80	0
1	OMU	2A	2563	21/22	0.95	0.28	59,75,95,110	0
1	5MC	1A	1963	21/22	0.96	0.18	37,53,70,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	5MU	1A	1960	21/22	0.96	0.28	40,55,69,75	0
1	OMU	1A	2563	21/22	0.96	0.22	35,43,54,63	0
1	2MA	1A	2514	23/24	0.97	0.23	24,40,53,58	0
1	5MU	2A	1960	21/22	0.97	0.27	54,66,78,79	0
1	PSU	1A	2616	20/21	0.97	0.21	30,41,57,57	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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
53	MG	1a	1902	1/1	-0.28	0.26	195,195,195,195	0
53	MG	1a	1846	1/1	-0.17	0.83	227,227,227,227	0
53	MG	2h	201	1/1	-0.12	1.12	123,123,123,123	0
53	MG	2a	1758	1/1	0.01	1.08	100,100,100,100	0
53	MG	2a	1786	1/1	0.03	0.43	91,91,91,91	0
53	MG	1A	3188	1/1	0.14	0.94	256,256,256,256	0
53	MG	1a	1754	1/1	0.14	0.93	95,95,95,95	0
53	MG	2A	3061	1/1	0.20	0.81	95,95,95,95	0
53	MG	1m	201	1/1	0.20	0.78	192,192,192,192	0
53	MG	2a	1713	1/1	0.24	2.40	119,119,119,119	0
53	MG	1a	1784	1/1	0.27	0.64	96,96,96,96	0
53	MG	2a	1722	1/1	0.27	1.24	161,161,161,161	0
53	MG	1a	1727	1/1	0.28	1.54	92,92,92,92	0
53	MG	2a	1755	1/1	0.29	1.05	120,120,120,120	0
53	MG	2a	1769	1/1	0.29	0.55	97,97,97,97	0
53	MG	2a	1773	1/1	0.30	0.25	141,141,141,141	0
53	MG	2a	1744	1/1	0.30	0.98	132,132,132,132	0
53	MG	2n	101	1/1	0.30	0.55	169,169,169,169	0
53	MG	1a	1770	1/1	0.33	0.72	81,81,81,81	0
53	MG	2A	3546	1/1	0.33	0.77	77,77,77,77	0
53	MG	1a	1748	1/1	0.34	0.65	107,107,107,107	0
53	MG	2A	3105	1/1	0.34	0.36	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	20	101	1/1	0.37	0.21	82,82,82,82	0
53	MG	2A	3098	1/1	0.38	0.59	90,90,90,90	0
53	MG	2a	1819	1/1	0.38	0.36	180,180,180,180	0
53	MG	1A	3525	1/1	0.39	0.73	108,108,108,108	0
53	MG	1a	1733	1/1	0.40	0.59	108,108,108,108	0
53	MG	1a	1904	1/1	0.40	0.16	240,240,240,240	0
53	MG	2A	3485	1/1	0.40	0.42	100,100,100,100	0
53	MG	1a	1716	1/1	0.41	1.24	179,179,179,179	0
53	MG	2A	3407	1/1	0.41	0.46	76,76,76,76	0
53	MG	1a	1867	1/1	0.43	0.40	143,143,143,143	0
53	MG	2A	3284	1/1	0.43	2.12	150,150,150,150	0
53	MG	1a	1819	1/1	0.46	0.66	124,124,124,124	0
53	MG	1f	8002	1/1	0.46	0.37	110,110,110,110	0
53	MG	2a	1732	1/1	0.46	0.59	188,188,188,188	0
53	MG	1a	1709	1/1	0.47	0.13	209,209,209,209	0
53	MG	2a	1745	1/1	0.47	0.27	79,79,79,79	0
53	MG	1A	3639	1/1	0.47	0.74	85,85,85,85	0
53	MG	1a	1858	1/1	0.47	0.49	152,152,152,152	0
53	MG	2A	3290	1/1	0.48	0.66	84,84,84,84	0
53	MG	2A	3414	1/1	0.48	0.17	116,116,116,116	0
53	MG	1a	1845	1/1	0.48	0.63	106,106,106,106	0
53	MG	2A	3236	1/1	0.49	0.46	110,110,110,110	0
53	MG	2A	3185	1/1	0.49	0.53	60,60,60,60	0
53	MG	2D	307	1/1	0.49	0.61	90,90,90,90	0
53	MG	1a	1865	1/1	0.49	0.47	78,78,78,78	0
53	MG	1a	1847	1/1	0.50	0.59	90,90,90,90	0
53	MG	2A	3128	1/1	0.51	0.46	97,97,97,97	0
53	MG	2a	1767	1/1	0.51	0.44	59,59,59,59	0
53	MG	2A	3070	1/1	0.51	0.64	83,83,83,83	0
53	MG	2a	1815	1/1	0.51	0.22	158,158,158,158	0
53	MG	2a	1754	1/1	0.52	0.37	83,83,83,83	0
53	MG	2a	1792	1/1	0.52	0.12	157,157,157,157	0
53	MG	1a	1817	1/1	0.52	0.34	122,122,122,122	0
53	MG	2a	1774	1/1	0.52	0.46	152,152,152,152	0
53	MG	2A	3543	1/1	0.52	0.60	91,91,91,91	0
53	MG	2I	3002	1/1	0.53	0.18	129,129,129,129	0
53	MG	2W	202	1/1	0.53	0.37	80,80,80,80	0
53	MG	2a	1757	1/1	0.53	0.78	206,206,206,206	0
53	MG	2a	1706	1/1	0.53	0.20	123,123,123,123	0
53	MG	1A	3124	1/1	0.54	0.53	82,82,82,82	0
53	MG	1a	1851	1/1	0.54	0.53	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	1A	3466	1/1	0.54	0.65	45,45,45,45	0
53	MG	2O	202	1/1	0.54	0.64	115,115,115,115	0
53	MG	1a	1746	1/1	0.55	0.20	167,167,167,167	0
53	MG	1B	206	1/1	0.56	0.30	75,75,75,75	0
53	MG	2A	3261	1/1	0.56	0.29	115,115,115,115	0
53	MG	2a	1783	1/1	0.56	0.96	183,183,183,183	0
53	MG	2A	3037	1/1	0.56	0.63	64,64,64,64	0
53	MG	2A	3348	1/1	0.56	0.67	114,114,114,114	0
53	MG	2a	1818	1/1	0.57	0.91	106,106,106,106	0
53	MG	2f	3001	1/1	0.57	0.30	87,87,87,87	0
53	MG	2A	3084	1/1	0.57	0.40	109,109,109,109	0
55	MPD	2B	210	8/8	0.57	0.44	114,144,150,162	0
53	MG	2A	3367	1/1	0.58	0.70	90,90,90,90	0
53	MG	1a	1767	1/1	0.58	0.26	99,99,99,99	0
53	MG	1A	3402	1/1	0.58	0.55	70,70,70,70	0
53	MG	2A	3469	1/1	0.59	0.49	109,109,109,109	0
53	MG	2a	1738	1/1	0.59	0.67	218,218,218,218	0
53	MG	2A	3518	1/1	0.59	0.58	91,91,91,91	0
53	MG	1Q	201	1/1	0.59	0.28	51,51,51,51	0
53	MG	1a	1717	1/1	0.59	0.54	196,196,196,196	0
53	MG	1a	1854	1/1	0.60	1.14	112,112,112,112	0
53	MG	1A	3777	1/1	0.60	0.60	93,93,93,93	0
53	MG	1a	1801	1/1	0.60	0.40	164,164,164,164	0
53	MG	1a	1796	1/1	0.60	0.37	119,119,119,119	0
53	MG	2A	3173	1/1	0.60	0.56	78,78,78,78	0
53	MG	2a	1727	1/1	0.60	1.28	149,149,149,149	0
53	MG	2A	3010	1/1	0.60	0.45	83,83,83,83	0
53	MG	1A	3087	1/1	0.60	0.32	94,94,94,94	0
53	MG	1a	1782	1/1	0.60	0.19	104,104,104,104	0
53	MG	2a	1770	1/1	0.61	0.13	141,141,141,141	0
53	MG	2A	3382	1/1	0.61	0.36	85,85,85,85	0
53	MG	2B	208	1/1	0.61	0.25	68,68,68,68	0
53	MG	2a	1760	1/1	0.62	0.35	81,81,81,81	0
53	MG	1A	3364	1/1	0.62	0.24	65,65,65,65	0
53	MG	2A	3134	1/1	0.62	0.30	69,69,69,69	0
53	MG	1A	3346	1/1	0.62	0.31	27,27,27,27	0
53	MG	1a	1872	1/1	0.62	0.42	78,78,78,78	0
53	MG	1A	3506	1/1	0.63	0.34	81,81,81,81	0
53	MG	2A	3005	1/1	0.63	0.56	87,87,87,87	0
53	MG	2A	3158	1/1	0.64	0.59	80,80,80,80	0
53	MG	2a	1703	1/1	0.64	0.57	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	2A	3511	1/1	0.64	0.20	132,132,132,132	0
53	MG	2A	3087	1/1	0.64	0.76	90,90,90,90	0
53	MG	1a	1726	1/1	0.64	0.30	91,91,91,91	0
53	MG	2a	1759	1/1	0.64	0.93	68,68,68,68	0
53	MG	2A	3510	1/1	0.64	0.42	77,77,77,77	0
53	MG	2t	3001	1/1	0.65	0.39	109,109,109,109	0
53	MG	2e	201	1/1	0.65	0.16	79,79,79,79	0
53	MG	1a	1785	1/1	0.65	0.66	72,72,72,72	0
53	MG	2A	3139	1/1	0.65	0.67	85,85,85,85	0
53	MG	1A	3634	1/1	0.65	0.30	52,52,52,52	0
53	MG	1a	1753	1/1	0.65	1.64	184,184,184,184	0
53	MG	1A	3665	1/1	0.65	0.92	74,74,74,74	0
53	MG	1A	3325	1/1	0.65	0.62	92,92,92,92	0
53	MG	2A	3212	1/1	0.66	0.75	59,59,59,59	0
53	MG	2X	101	1/1	0.66	0.70	70,70,70,70	0
53	MG	2A	3539	1/1	0.66	0.50	78,78,78,78	0
53	MG	2A	3525	1/1	0.66	0.50	106,106,106,106	0
53	MG	1A	3769	1/1	0.66	0.43	71,71,71,71	0
53	MG	2A	3460	1/1	0.66	0.60	128,128,128,128	0
53	MG	2a	1794	1/1	0.66	1.36	84,84,84,84	0
53	MG	1A	3482	1/1	0.66	0.52	81,81,81,81	0
53	MG	2l	201	1/1	0.66	0.29	89,89,89,89	0
53	MG	1A	3075	1/1	0.67	0.34	83,83,83,83	0
53	MG	2A	3519	1/1	0.67	0.32	87,87,87,87	0
53	MG	1a	1714	1/1	0.67	0.69	211,211,211,211	0
53	MG	2A	3495	1/1	0.67	0.40	69,69,69,69	0
53	MG	1a	1776	1/1	0.67	0.36	88,88,88,88	0
53	MG	2A	3342	1/1	0.67	0.25	86,86,86,86	0
53	MG	1e	3001	1/1	0.67	0.24	89,89,89,89	0
53	MG	2a	1707	1/1	0.67	1.07	76,76,76,76	0
53	MG	2A	3013	1/1	0.67	0.40	79,79,79,79	0
53	MG	2r	101	1/1	0.68	0.53	95,95,95,95	0
53	MG	1a	1736	1/1	0.68	0.79	87,87,87,87	0
53	MG	1A	3545	1/1	0.68	0.43	72,72,72,72	0
53	MG	1A	3576	1/1	0.68	0.40	75,75,75,75	0
53	MG	1A	3042	1/1	0.68	0.74	87,87,87,87	0
53	MG	2a	1812	1/1	0.68	0.52	86,86,86,86	0
53	MG	2a	1840	1/1	0.68	0.56	86,86,86,86	0
53	MG	2A	3341	1/1	0.68	0.23	117,117,117,117	0
53	MG	2A	3054	1/1	0.69	0.35	142,142,142,142	0
53	MG	2a	1789	1/1	0.69	0.67	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	2a	1824	1/1	0.69	0.39	108,108,108,108	0
53	MG	1A	3772	1/1	0.69	0.57	98,98,98,98	0
53	MG	1A	3741	1/1	0.69	0.71	84,84,84,84	0
53	MG	1a	1897	1/1	0.69	0.33	88,88,88,88	0
53	MG	1A	3088	1/1	0.69	0.30	66,66,66,66	0
53	MG	1A	3494	1/1	0.69	0.30	86,86,86,86	0
53	MG	1a	1881	1/1	0.69	1.73	99,99,99,99	0
53	MG	2A	3376	1/1	0.69	0.79	108,108,108,108	0
53	MG	1A	3154	1/1	0.69	0.57	76,76,76,76	0
53	MG	1A	3611	1/1	0.70	0.15	102,102,102,102	0
53	MG	1A	3055	1/1	0.70	0.48	56,56,56,56	0
53	MG	1A	3110	1/1	0.70	0.32	109,109,109,109	0
53	MG	1A	3811	1/1	0.70	0.17	72,72,72,72	0
53	MG	1A	3129	1/1	0.70	1.15	91,91,91,91	0
53	MG	1A	3565	1/1	0.70	0.11	105,105,105,105	0
53	MG	2A	3024	1/1	0.70	0.41	86,86,86,86	0
53	MG	2a	1804	1/1	0.70	0.62	151,151,151,151	0
53	MG	1a	1821	1/1	0.71	0.49	130,130,130,130	0
53	MG	1B	213	1/1	0.71	0.48	97,97,97,97	0
53	MG	2a	1746	1/1	0.71	0.24	67,67,67,67	0
53	MG	2a	1740	1/1	0.71	0.42	85,85,85,85	0
53	MG	1a	1704	1/1	0.71	0.27	193,193,193,193	0
53	MG	2A	3266	1/1	0.71	0.37	55,55,55,55	0
53	MG	1A	3542	1/1	0.71	0.42	98,98,98,98	0
53	MG	2A	3063	1/1	0.71	0.37	86,86,86,86	0
53	MG	1A	3664	1/1	0.71	0.21	62,62,62,62	0
53	MG	1A	3752	1/1	0.71	0.67	61,61,61,61	0
53	MG	1a	1859	1/1	0.72	0.26	105,105,105,105	0
53	MG	2a	1842	1/1	0.72	0.21	98,98,98,98	0
53	MG	2A	3035	1/1	0.72	0.40	90,90,90,90	0
53	MG	2P	201	1/1	0.72	0.37	81,81,81,81	0
53	MG	2A	3443	1/1	0.72	0.15	91,91,91,91	0
53	MG	1a	1715	1/1	0.72	0.14	236,236,236,236	0
53	MG	2B	206	1/1	0.72	0.62	71,71,71,71	0
53	MG	2A	3120	1/1	0.72	0.37	66,66,66,66	0
53	MG	2A	3069	1/1	0.72	0.30	75,75,75,75	0
53	MG	2a	1816	1/1	0.72	0.28	100,100,100,100	0
53	MG	1s	101	1/1	0.72	0.09	158,158,158,158	0
53	MG	2A	3017	1/1	0.72	0.31	69,69,69,69	0
53	MG	2a	1714	1/1	0.73	0.30	106,106,106,106	0
53	MG	1W	3002	1/1	0.73	0.54	45,45,45,45	0
53	MG	1a	1831	1/1	0.73	0.29	110,110,110,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	1a	1837	1/1	0.73	0.19	97,97,97,97	0
53	MG	2a	1833	1/1	0.73	0.63	85,85,85,85	0
53	MG	1Q	202	1/1	0.73	0.44	80,80,80,80	0
53	MG	1a	1718	1/1	0.73	0.22	193,193,193,193	0
53	MG	2a	1721	1/1	0.73	0.40	72,72,72,72	0
53	MG	1A	3413	1/1	0.73	0.46	57,57,57,57	0
53	MG	1t	3001	1/1	0.73	0.51	92,92,92,92	0
53	MG	1A	3548	1/1	0.73	0.84	118,118,118,118	0
53	MG	1A	3113	1/1	0.73	0.31	59,59,59,59	0
53	MG	2A	3507	1/1	0.73	0.37	92,92,92,92	0
53	MG	1A	3710	1/1	0.73	0.14	68,68,68,68	0
53	MG	2a	1801	1/1	0.73	0.73	72,72,72,72	0
53	MG	1a	1747	1/1	0.73	0.34	64,64,64,64	0
53	MG	2A	3188	1/1	0.73	0.23	79,79,79,79	0
53	MG	2A	3197	1/1	0.73	0.72	73,73,73,73	0
53	MG	1A	3826	1/1	0.73	0.26	52,52,52,52	0
53	MG	2A	3163	1/1	0.73	0.23	75,75,75,75	0
53	MG	2A	3500	1/1	0.73	0.46	99,99,99,99	0
53	MG	1A	3478	1/1	0.73	0.44	59,59,59,59	0
53	MG	1A	3296	1/1	0.73	1.13	61,61,61,61	0
53	MG	1A	3530	1/1	0.74	0.71	74,74,74,74	0
53	MG	2a	1832	1/1	0.74	0.44	76,76,76,76	0
53	MG	1a	1707	1/1	0.74	0.23	75,75,75,75	0
53	MG	2a	1743	1/1	0.74	1.07	98,98,98,98	0
53	MG	2A	3025	1/1	0.74	0.24	85,85,85,85	0
53	MG	1A	3142	1/1	0.74	0.23	75,75,75,75	0
53	MG	1a	1755	1/1	0.74	0.23	87,87,87,87	0
53	MG	2A	3484	1/1	0.74	0.22	81,81,81,81	0
53	MG	2a	1761	1/1	0.74	0.26	90,90,90,90	0
53	MG	1a	1848	1/1	0.74	0.14	107,107,107,107	0
53	MG	1a	1810	1/1	0.74	0.41	211,211,211,211	0
53	MG	1A	3531	1/1	0.74	0.48	61,61,61,61	0
53	MG	2a	1836	1/1	0.74	0.34	83,83,83,83	0
53	MG	1A	3601	1/1	0.75	0.49	56,56,56,56	0
53	MG	1A	3600	1/1	0.75	0.42	58,58,58,58	0
53	MG	1A	3521	1/1	0.75	0.36	58,58,58,58	0
53	MG	1a	1820	1/1	0.75	0.35	107,107,107,107	0
53	MG	2A	3068	1/1	0.75	0.44	68,68,68,68	0
53	MG	1B	221	1/1	0.75	0.77	80,80,80,80	0
53	MG	1A	3755	1/1	0.75	0.29	79,79,79,79	0
53	MG	2a	1777	1/1	0.75	0.51	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	1a	1731	1/1	0.75	0.24	78,78,78,78	0
53	MG	2A	3205	1/1	0.75	0.71	81,81,81,81	0
53	MG	2A	3085	1/1	0.75	0.19	123,123,123,123	0
53	MG	1a	1781	1/1	0.75	0.80	123,123,123,123	0
53	MG	1A	3712	1/1	0.75	0.48	79,79,79,79	0
53	MG	1a	1745	1/1	0.75	0.27	71,71,71,71	0
53	MG	2A	3248	1/1	0.75	0.25	103,103,103,103	0
53	MG	2A	3230	1/1	0.75	0.40	87,87,87,87	0
53	MG	2A	3465	1/1	0.76	0.36	74,74,74,74	0
53	MG	2a	1781	1/1	0.76	0.37	85,85,85,85	0
53	MG	1A	3518	1/1	0.76	0.13	92,92,92,92	0
53	MG	2A	3328	1/1	0.76	0.28	89,89,89,89	0
53	MG	1A	3130	1/1	0.76	1.17	100,100,100,100	0
53	MG	2A	3106	1/1	0.76	0.28	74,74,74,74	0
53	MG	1A	3376	1/1	0.76	0.24	70,70,70,70	0
53	MG	1A	3319	1/1	0.76	0.13	79,79,79,79	0
53	MG	2A	3174	1/1	0.76	0.14	75,75,75,75	0
53	MG	1A	3049	1/1	0.76	0.50	84,84,84,84	0
53	MG	1A	3440	1/1	0.76	0.28	60,60,60,60	0
53	MG	2a	1756	1/1	0.76	0.38	92,92,92,92	0
53	MG	1a	1874	1/1	0.76	0.31	51,51,51,51	0
53	MG	2a	1753	1/1	0.76	0.31	127,127,127,127	0
53	MG	1l	102	1/1	0.76	0.33	70,70,70,70	0
53	MG	1A	3524	1/1	0.76	0.16	79,79,79,79	0
53	MG	2A	3304	1/1	0.76	0.36	78,78,78,78	0
53	MG	1a	1735	1/1	0.76	0.43	207,207,207,207	0
53	MG	1A	3293	1/1	0.77	0.49	83,83,83,83	0
53	MG	1B	224	1/1	0.77	0.23	82,82,82,82	0
53	MG	1A	3388	1/1	0.77	0.45	72,72,72,72	0
53	MG	2P	202	1/1	0.77	0.40	85,85,85,85	0
53	MG	2a	1716	1/1	0.77	0.07	112,112,112,112	0
53	MG	2A	3117	1/1	0.77	0.71	69,69,69,69	0
53	MG	2A	3118	1/1	0.77	0.31	76,76,76,76	0
53	MG	2A	3541	1/1	0.77	0.24	57,57,57,57	0
53	MG	2A	3468	1/1	0.77	0.19	93,93,93,93	0
53	MG	2a	1737	1/1	0.77	0.53	85,85,85,85	0
53	MG	1A	3643	1/1	0.77	0.25	46,46,46,46	0
53	MG	1A	3114	1/1	0.77	0.50	76,76,76,76	0
53	MG	2a	1730	1/1	0.77	0.37	87,87,87,87	0
53	MG	1a	1788	1/1	0.77	0.28	83,83,83,83	0
53	MG	1T	8002	1/1	0.77	0.93	94,94,94,94	0
53	MG	2A	3325	1/1	0.77	0.51	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	1D	303	1/1	0.77	0.73	79,79,79,79	0
53	MG	2a	1708	1/1	0.77	0.19	129,129,129,129	0
53	MG	1A	3165	1/1	0.77	0.47	83,83,83,83	0
53	MG	2a	1718	1/1	0.77	0.12	89,89,89,89	0
53	MG	2a	1710	1/1	0.77	0.29	119,119,119,119	0
53	MG	28	8002	1/1	0.77	0.70	74,74,74,74	0
53	MG	2A	3313	1/1	0.77	0.13	91,91,91,91	0
53	MG	1a	1891	1/1	0.77	1.00	67,67,67,67	0
53	MG	1A	3102	1/1	0.77	0.35	72,72,72,72	0
53	MG	1B	220	1/1	0.77	0.36	53,53,53,53	0
53	MG	2A	3113	1/1	0.77	0.36	96,96,96,96	0
53	MG	2A	3219	1/1	0.77	0.71	100,100,100,100	0
53	MG	2A	3540	1/1	0.78	0.40	82,82,82,82	0
53	MG	2a	1806	1/1	0.78	0.33	85,85,85,85	0
53	MG	1a	1852	1/1	0.78	0.41	70,70,70,70	0
53	MG	1A	3302	1/1	0.78	0.39	63,63,63,63	0
53	MG	1A	3032	1/1	0.78	0.35	65,65,65,65	0
53	MG	1F	306	1/1	0.78	0.43	75,75,75,75	0
53	MG	2Q	8001	1/1	0.78	0.39	72,72,72,72	0
53	MG	2A	3088	1/1	0.78	1.04	58,58,58,58	0
53	MG	2A	3322	1/1	0.78	0.31	114,114,114,114	0
53	MG	2A	3123	1/1	0.78	0.27	66,66,66,66	0
53	MG	1A	3594	1/1	0.78	0.30	80,80,80,80	0
53	MG	1a	1836	1/1	0.78	0.17	98,98,98,98	0
53	MG	1A	3417	1/1	0.78	0.28	96,96,96,96	0
53	MG	1D	312	1/1	0.78	0.39	57,57,57,57	0
53	MG	2a	1837	1/1	0.78	0.60	78,78,78,78	0
53	MG	1A	3002	1/1	0.78	0.62	60,60,60,60	0
53	MG	1B	225	1/1	0.78	0.97	69,69,69,69	0
53	MG	1A	3632	1/1	0.78	0.74	44,44,44,44	0
53	MG	2A	3461	1/1	0.78	0.32	95,95,95,95	0
53	MG	1A	3781	1/1	0.78	0.44	33,33,33,33	0
53	MG	1a	1744	1/1	0.78	0.42	69,69,69,69	0
53	MG	1A	3175	1/1	0.78	0.36	86,86,86,86	0
53	MG	1a	1838	1/1	0.78	0.32	67,67,67,67	0
53	MG	1A	3557	1/1	0.79	0.97	64,64,64,64	0
53	MG	1A	3222	1/1	0.79	0.33	46,46,46,46	0
53	MG	1a	1857	1/1	0.79	0.91	122,122,122,122	0
53	MG	1A	3282	1/1	0.79	0.39	52,52,52,52	0
53	MG	2A	3368	1/1	0.79	0.41	75,75,75,75	0
53	MG	1a	1815	1/1	0.79	0.24	78,78,78,78	0
53	MG	1A	3146	1/1	0.79	0.34	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	1A	3182	1/1	0.79	0.40	74,74,74,74	0
53	MG	1h	3001	1/1	0.79	0.96	74,74,74,74	0
53	MG	1A	3044	1/1	0.79	1.28	88,88,88,88	0
53	MG	1A	3615	1/1	0.79	0.20	69,69,69,69	0
53	MG	1A	3336	1/1	0.79	0.29	44,44,44,44	0
53	MG	2A	3177	1/1	0.79	0.25	70,70,70,70	0
53	MG	1A	3606	1/1	0.79	0.63	60,60,60,60	0
53	MG	1A	3473	1/1	0.79	0.71	62,62,62,62	0
53	MG	1A	3593	1/1	0.79	0.31	62,62,62,62	0
53	MG	1A	3097	1/1	0.79	0.81	64,64,64,64	0
53	MG	1A	3630	1/1	0.79	0.50	57,57,57,57	0
53	MG	1a	1758	1/1	0.79	0.16	152,152,152,152	0
53	MG	1A	3648	1/1	0.80	0.21	63,63,63,63	0
53	MG	2A	3077	1/1	0.80	0.42	86,86,86,86	0
53	MG	2a	1749	1/1	0.80	0.30	75,75,75,75	0
53	MG	1A	3555	1/1	0.80	0.48	93,93,93,93	0
53	MG	2A	3392	1/1	0.80	0.21	66,66,66,66	0
53	MG	2A	3359	1/1	0.80	0.08	78,78,78,78	0
53	MG	2A	3265	1/1	0.80	0.34	72,72,72,72	0
53	MG	2A	3474	1/1	0.80	0.27	102,102,102,102	0
53	MG	2A	3389	1/1	0.80	0.29	75,75,75,75	0
53	MG	1A	3169	1/1	0.80	0.35	88,88,88,88	0
53	MG	1A	3493	1/1	0.80	0.73	110,110,110,110	0
53	MG	2A	3103	1/1	0.80	0.50	96,96,96,96	0
53	MG	2a	1782	1/1	0.80	0.31	78,78,78,78	0
53	MG	1A	3540	1/1	0.80	0.43	67,67,67,67	0
53	MG	2A	3032	1/1	0.80	0.74	69,69,69,69	0
53	MG	2A	3544	1/1	0.80	0.31	59,59,59,59	0
53	MG	1A	3770	1/1	0.80	0.26	85,85,85,85	0
53	MG	2A	3064	1/1	0.80	0.17	91,91,91,91	0
53	MG	1A	3187	1/1	0.80	0.26	65,65,65,65	0
53	MG	1a	1892	1/1	0.80	0.34	91,91,91,91	0
55	MPD	2A	3552	8/8	0.80	0.34	72,112,120,128	0
53	MG	1A	3137	1/1	0.80	0.33	66,66,66,66	0
53	MG	1a	1713	1/1	0.80	0.20	81,81,81,81	0
53	MG	2E	305	1/1	0.80	0.16	83,83,83,83	0
53	MG	1A	3270	1/1	0.80	0.28	50,50,50,50	0
53	MG	1a	1724	1/1	0.80	0.24	63,63,63,63	0
53	MG	2A	3536	1/1	0.80	0.20	90,90,90,90	0
53	MG	1A	3377	1/1	0.80	0.60	79,79,79,79	0
53	MG	2a	1822	1/1	0.80	0.36	101,101,101,101	0
53	MG	1A	3754	1/1	0.80	0.25	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	2A	3272	1/1	0.80	0.24	114,114,114,114	0
53	MG	2A	3119	1/1	0.80	0.18	129,129,129,129	0
53	MG	1A	3636	1/1	0.80	0.26	48,48,48,48	0
53	MG	1a	1868	1/1	0.81	0.58	128,128,128,128	0
53	MG	1A	3638	1/1	0.81	0.43	65,65,65,65	0
53	MG	2A	3340	1/1	0.81	0.15	64,64,64,64	0
53	MG	1A	3793	1/1	0.81	0.63	60,60,60,60	0
53	MG	2A	3109	1/1	0.81	0.25	89,89,89,89	0
53	MG	1A	3763	1/1	0.81	0.33	69,69,69,69	0
53	MG	1A	3083	1/1	0.81	0.18	58,58,58,58	0
53	MG	1A	3588	1/1	0.81	0.11	77,77,77,77	0
53	MG	1G	8001	1/1	0.81	0.07	95,95,95,95	0
53	MG	2A	3130	1/1	0.81	0.45	73,73,73,73	0
53	MG	1A	3653	1/1	0.81	0.53	59,59,59,59	0
53	MG	2A	3125	1/1	0.81	0.34	114,114,114,114	0
53	MG	1a	1866	1/1	0.81	0.34	68,68,68,68	0
53	MG	1a	1826	1/1	0.81	0.33	99,99,99,99	0
53	MG	1A	3732	1/1	0.81	0.48	62,62,62,62	0
53	MG	1A	3616	1/1	0.81	0.24	73,73,73,73	0
53	MG	1A	3758	1/1	0.81	0.23	53,53,53,53	0
53	MG	1A	3624	1/1	0.81	0.44	74,74,74,74	0
53	MG	1a	1719	1/1	0.81	0.36	224,224,224,224	0
53	MG	2f	3002	1/1	0.81	0.28	74,74,74,74	0
53	MG	2A	3347	1/1	0.81	0.28	80,80,80,80	0
53	MG	1H	202	1/1	0.81	0.32	61,61,61,61	0
53	MG	1F	303	1/1	0.81	0.38	56,56,56,56	0
53	MG	2A	3315	1/1	0.81	0.77	64,64,64,64	0
53	MG	2A	3111	1/1	0.81	0.13	138,138,138,138	0
53	MG	2A	3559	1/1	0.81	0.21	78,78,78,78	0
53	MG	2A	3094	1/1	0.81	0.27	117,117,117,117	0
53	MG	2A	3424	1/1	0.81	0.31	77,77,77,77	0
53	MG	1A	3263	1/1	0.81	0.21	47,47,47,47	0
53	MG	2a	1717	1/1	0.81	0.38	100,100,100,100	0
53	MG	1a	1775	1/1	0.81	0.64	74,74,74,74	0
53	MG	1A	3086	1/1	0.81	0.27	77,77,77,77	0
53	MG	1A	3689	1/1	0.81	0.26	69,69,69,69	0
53	MG	2A	3062	1/1	0.81	0.22	118,118,118,118	0
53	MG	2A	3273	1/1	0.81	0.36	70,70,70,70	0
53	MG	2a	1731	1/1	0.81	0.17	92,92,92,92	0
53	MG	2A	3381	1/1	0.81	0.32	67,67,67,67	0
53	MG	1A	3717	1/1	0.81	0.17	72,72,72,72	0
57	ZN	2n	102	1/1	0.81	0.12	205,205,205,205	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	2a	1779	1/1	0.81	0.13	109,109,109,109	0
53	MG	1A	3731	1/1	0.81	0.18	86,86,86,86	0
53	MG	10	104	1/1	0.81	0.13	70,70,70,70	0
53	MG	1G	8003	1/1	0.81	0.11	92,92,92,92	0
53	MG	2A	3133	1/1	0.81	0.42	84,84,84,84	0
53	MG	1a	1839	1/1	0.81	0.46	121,121,121,121	0
53	MG	2A	3366	1/1	0.82	0.38	86,86,86,86	0
53	MG	2A	3334	1/1	0.82	0.20	64,64,64,64	0
53	MG	2A	3550	1/1	0.82	0.48	61,61,61,61	0
53	MG	2A	3232	1/1	0.82	0.31	76,76,76,76	0
53	MG	2A	3224	1/1	0.82	0.24	92,92,92,92	0
53	MG	2A	3388	1/1	0.82	0.26	63,63,63,63	0
53	MG	11	103	1/1	0.82	0.35	61,61,61,61	0
55	MPD	2A	3551	8/8	0.82	0.40	57,89,97,104	0
53	MG	1F	308	1/1	0.82	0.56	52,52,52,52	0
53	MG	2A	3293	1/1	0.82	0.92	68,68,68,68	0
53	MG	1a	1896	1/1	0.82	0.71	100,100,100,100	0
53	MG	1A	3301	1/1	0.82	0.48	53,53,53,53	0
53	MG	1A	3419	1/1	0.82	0.33	38,38,38,38	0
53	MG	1A	3737	1/1	0.82	0.16	73,73,73,73	0
53	MG	2A	3409	1/1	0.82	0.52	59,59,59,59	0
53	MG	1A	3779	1/1	0.82	0.28	71,71,71,71	0
53	MG	2a	1791	1/1	0.82	0.07	114,114,114,114	0
53	MG	2A	3031	1/1	0.82	0.30	82,82,82,82	0
53	MG	2A	3471	1/1	0.82	0.26	51,51,51,51	0
53	MG	1a	1792	1/1	0.82	0.29	71,71,71,71	0
53	MG	1A	3642	1/1	0.82	0.15	77,77,77,77	0
53	MG	1A	3298	1/1	0.82	0.35	73,73,73,73	0
53	MG	1A	3024	1/1	0.82	0.74	91,91,91,91	0
53	MG	2B	205	1/1	0.82	0.27	62,62,62,62	0
53	MG	2A	3116	1/1	0.82	0.40	68,68,68,68	0
53	MG	2a	1831	1/1	0.82	0.64	55,55,55,55	0
53	MG	2A	3415	1/1	0.82	0.24	81,81,81,81	0
53	MG	2A	3448	1/1	0.82	0.16	120,120,120,120	0
53	MG	1A	3706	1/1	0.82	0.15	44,44,44,44	0
53	MG	1A	3163	1/1	0.83	0.88	75,75,75,75	0
53	MG	1A	3485	1/1	0.83	0.21	80,80,80,80	0
53	MG	2F	301	1/1	0.83	0.23	72,72,72,72	0
53	MG	1A	3736	1/1	0.83	0.25	53,53,53,53	0
53	MG	2a	1796	1/1	0.83	0.27	93,93,93,93	0
53	MG	1a	1729	1/1	0.83	0.11	96,96,96,96	0
53	MG	2A	3121	1/1	0.83	0.17	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	1A	3248	1/1	0.83	0.37	63,63,63,63	0
53	MG	1A	3201	1/1	0.83	0.35	41,41,41,41	0
53	MG	1A	3207	1/1	0.83	0.22	52,52,52,52	0
53	MG	1a	1725	1/1	0.83	0.28	55,55,55,55	0
53	MG	1A	3090	1/1	0.83	0.41	66,66,66,66	0
53	MG	2a	1712	1/1	0.83	0.23	109,109,109,109	0
53	MG	2A	3516	1/1	0.83	0.31	78,78,78,78	0
53	MG	2a	1711	1/1	0.83	0.32	84,84,84,84	0
53	MG	1A	3159	1/1	0.83	0.27	88,88,88,88	0
53	MG	2A	3462	1/1	0.83	0.27	88,88,88,88	0
53	MG	2E	302	1/1	0.83	0.22	106,106,106,106	0
53	MG	2A	3280	1/1	0.83	0.32	70,70,70,70	0
53	MG	2A	3311	1/1	0.83	0.44	63,63,63,63	0
53	MG	2A	3444	1/1	0.83	0.27	54,54,54,54	0
53	MG	1A	3511	1/1	0.83	0.26	77,77,77,77	0
53	MG	1A	3432	1/1	0.83	0.26	79,79,79,79	0
53	MG	2a	1793	1/1	0.83	0.35	87,87,87,87	0
55	MPD	1T	8004	8/8	0.83	0.28	85,109,114,114	0
53	MG	1A	3399	1/1	0.83	0.19	50,50,50,50	0
53	MG	2A	3439	1/1	0.83	0.16	54,54,54,54	0
53	MG	1a	1877	1/1	0.83	0.56	87,87,87,87	0
53	MG	2A	3523	1/1	0.83	0.17	69,69,69,69	0
53	MG	17	102	1/1	0.83	0.42	56,56,56,56	0
53	MG	2A	3180	1/1	0.83	0.40	60,60,60,60	0
53	MG	1a	1759	1/1	0.83	0.14	73,73,73,73	0
53	MG	2A	3115	1/1	0.83	0.37	105,105,105,105	0
53	MG	1A	3750	1/1	0.83	0.27	78,78,78,78	0
53	MG	1A	3093	1/1	0.83	0.16	71,71,71,71	0
53	MG	1A	3026	1/1	0.83	0.27	71,71,71,71	0
53	MG	2A	3076	1/1	0.83	0.31	61,61,61,61	0
53	MG	1A	3429	1/1	0.84	0.17	50,50,50,50	0
53	MG	2a	1768	1/1	0.84	0.21	89,89,89,89	0
53	MG	2A	3505	1/1	0.84	0.73	99,99,99,99	0
53	MG	1B	222	1/1	0.84	0.18	69,69,69,69	0
53	MG	1A	3276	1/1	0.84	0.15	68,68,68,68	0
53	MG	1A	3610	1/1	0.84	0.38	66,66,66,66	0
53	MG	28	8004	1/1	0.84	0.24	63,63,63,63	0
53	MG	2A	3276	1/1	0.84	0.24	73,73,73,73	0
53	MG	2B	207	1/1	0.84	0.17	67,67,67,67	0
53	MG	1A	3156	1/1	0.84	1.09	76,76,76,76	0
53	MG	1o	3001	1/1	0.84	0.32	51,51,51,51	0
53	MG	1a	1734	1/1	0.84	0.39	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	2A	3249	1/1	0.84	0.20	79,79,79,79	0
53	MG	2r	102	1/1	0.84	0.14	104,104,104,104	0
53	MG	1A	3629	1/1	0.84	0.55	44,44,44,44	0
53	MG	1A	3782	1/1	0.84	0.81	66,66,66,66	0
53	MG	2A	3007	1/1	0.84	0.28	61,61,61,61	0
53	MG	2A	3457	1/1	0.84	0.56	94,94,94,94	0
53	MG	2E	303	1/1	0.84	0.36	79,79,79,79	0
53	MG	1a	1711	1/1	0.84	0.19	90,90,90,90	0
53	MG	1A	3727	1/1	0.84	0.10	82,82,82,82	0
53	MG	2A	3499	1/1	0.84	0.17	70,70,70,70	0
53	MG	1A	3541	1/1	0.84	0.53	78,78,78,78	0
53	MG	2A	3198	1/1	0.84	0.27	66,66,66,66	0
53	MG	1A	3569	1/1	0.84	0.30	69,69,69,69	0
53	MG	2a	1725	1/1	0.84	0.22	93,93,93,93	0
53	MG	1A	3666	1/1	0.84	0.29	91,91,91,91	0
53	MG	2A	3038	1/1	0.84	0.47	55,55,55,55	0
53	MG	2a	1766	1/1	0.84	0.59	119,119,119,119	0
53	MG	1A	3384	1/1	0.84	0.48	70,70,70,70	0
53	MG	2A	3141	1/1	0.84	0.41	72,72,72,72	0
53	MG	2A	3263	1/1	0.84	0.28	72,72,72,72	0
53	MG	2l	202	1/1	0.84	0.98	73,73,73,73	0
53	MG	1A	3289	1/1	0.84	0.17	61,61,61,61	0
53	MG	1A	3787	1/1	0.84	0.32	86,86,86,86	0
53	MG	2A	3153	1/1	0.84	0.80	71,71,71,71	0
53	MG	1A	3751	1/1	0.84	0.69	82,82,82,82	0
53	MG	1a	1708	1/1	0.84	0.08	164,164,164,164	0
53	MG	1a	1812	1/1	0.84	0.16	93,93,93,93	0
53	MG	2A	3262	1/1	0.84	0.15	89,89,89,89	0
53	MG	2A	3475	1/1	0.84	0.10	83,83,83,83	0
53	MG	2a	1778	1/1	0.84	0.45	111,111,111,111	0
53	MG	1A	3240	1/1	0.84	0.33	101,101,101,101	0
54	ARG	1A	3799	12/12	0.84	0.28	85,101,112,114	0
53	MG	1a	1829	1/1	0.84	0.15	64,64,64,64	0
53	MG	2A	3148	1/1	0.84	0.51	76,76,76,76	0
53	MG	2A	3099	1/1	0.84	0.36	105,105,105,105	0
53	MG	10	105	1/1	0.84	0.23	68,68,68,68	0
53	MG	2A	3124	1/1	0.84	1.08	69,69,69,69	0
53	MG	1A	3460	1/1	0.84	0.29	66,66,66,66	0
53	MG	2A	3446	1/1	0.84	0.25	115,115,115,115	0
53	MG	1a	1856	1/1	0.84	0.12	109,109,109,109	0
53	MG	2E	304	1/1	0.84	0.14	93,93,93,93	0
53	MG	1a	1710	1/1	0.84	0.77	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	2A	3285	1/1	0.84	1.04	78,78,78,78	0
53	MG	1A	3471	1/1	0.84	0.30	29,29,29,29	0
53	MG	2a	1776	1/1	0.84	1.06	157,157,157,157	0
53	MG	2a	1733	1/1	0.84	0.14	171,171,171,171	0
53	MG	1A	3117	1/1	0.85	0.55	85,85,85,85	0
53	MG	2A	3131	1/1	0.85	0.55	69,69,69,69	0
53	MG	1B	201	1/1	0.85	0.21	48,48,48,48	0
53	MG	1A	3637	1/1	0.85	0.32	74,74,74,74	0
53	MG	2a	1762	1/1	0.85	0.20	88,88,88,88	0
53	MG	2a	1715	1/1	0.85	0.18	168,168,168,168	0
53	MG	2A	3066	1/1	0.85	0.23	92,92,92,92	0
53	MG	2A	3194	1/1	0.85	0.79	75,75,75,75	0
53	MG	1A	3721	1/1	0.85	0.33	84,84,84,84	0
53	MG	2a	1772	1/1	0.85	0.38	70,70,70,70	0
53	MG	2a	1798	1/1	0.85	0.23	98,98,98,98	0
53	MG	2A	3295	1/1	0.85	0.27	78,78,78,78	0
53	MG	1D	306	1/1	0.85	0.21	49,49,49,49	0
53	MG	1A	3018	1/1	0.85	0.62	70,70,70,70	0
53	MG	2a	1839	1/1	0.85	0.43	73,73,73,73	0
53	MG	2A	3426	1/1	0.85	0.26	86,86,86,86	0
53	MG	1a	1855	1/1	0.85	0.12	71,71,71,71	0
53	MG	1A	3469	1/1	0.85	0.26	59,59,59,59	0
53	MG	1A	3635	1/1	0.85	0.41	45,45,45,45	0
53	MG	1a	1811	1/1	0.85	0.25	61,61,61,61	0
53	MG	1d	502	1/1	0.85	0.53	66,66,66,66	0
53	MG	1a	1778	1/1	0.85	0.16	68,68,68,68	0
53	MG	1A	3683	1/1	0.85	0.39	62,62,62,62	0
53	MG	2A	3018	1/1	0.85	0.26	139,139,139,139	0
53	MG	1A	3371	1/1	0.85	0.42	70,70,70,70	0
53	MG	2A	3151	1/1	0.85	0.23	83,83,83,83	0
53	MG	10	103	1/1	0.85	0.44	84,84,84,84	0
53	MG	2a	1825	1/1	0.85	0.51	90,90,90,90	0
53	MG	1A	3461	1/1	0.85	1.05	87,87,87,87	0
53	MG	1A	3509	1/1	0.85	0.47	85,85,85,85	0
53	MG	2A	3497	1/1	0.85	0.29	75,75,75,75	0
53	MG	18	102	1/1	0.85	0.93	75,75,75,75	0
53	MG	2A	3149	1/1	0.85	0.46	81,81,81,81	0
53	MG	1F	301	1/1	0.85	0.44	73,73,73,73	0
53	MG	1A	3708	1/1	0.85	0.52	90,90,90,90	0
53	MG	2U	202	1/1	0.85	0.22	81,81,81,81	0
53	MG	1A	3421	1/1	0.85	0.20	74,74,74,74	0
53	MG	1D	307	1/1	0.85	0.40	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	2A	3537	1/1	0.85	0.91	65,65,65,65	0
53	MG	2A	3092	1/1	0.85	0.23	72,72,72,72	0
53	MG	1A	3702	1/1	0.85	0.37	83,83,83,83	0
53	MG	2A	3056	1/1	0.85	0.38	92,92,92,92	0
53	MG	2a	1734	1/1	0.85	0.23	78,78,78,78	0
53	MG	2A	3464	1/1	0.85	0.32	90,90,90,90	0
53	MG	1A	3321	1/1	0.85	0.45	55,55,55,55	0
53	MG	1A	3266	1/1	0.85	0.23	28,28,28,28	0
53	MG	1V	202	1/1	0.85	0.36	77,77,77,77	0
53	MG	1T	8003	1/1	0.86	0.30	89,89,89,89	0
53	MG	1V	201	1/1	0.86	0.31	60,60,60,60	0
53	MG	2A	3357	1/1	0.86	0.59	107,107,107,107	0
53	MG	2I	3001	1/1	0.86	0.25	159,159,159,159	0
53	MG	2A	3091	1/1	0.86	0.18	73,73,73,73	0
53	MG	2A	3053	1/1	0.86	0.27	98,98,98,98	0
53	MG	2B	209	1/1	0.86	0.10	87,87,87,87	0
53	MG	1a	1768	1/1	0.86	0.43	172,172,172,172	0
53	MG	1A	3309	1/1	0.86	0.30	104,104,104,104	0
53	MG	2A	3234	1/1	0.86	0.10	79,79,79,79	0
53	MG	1A	3464	1/1	0.86	0.32	90,90,90,90	0
53	MG	2B	203	1/1	0.86	0.69	85,85,85,85	0
53	MG	2a	1701	1/1	0.86	0.26	74,74,74,74	0
53	MG	2A	3379	1/1	0.86	0.22	114,114,114,114	0
53	MG	2a	1728	1/1	0.86	0.35	98,98,98,98	0
53	MG	1A	3463	1/1	0.86	0.27	58,58,58,58	0
53	MG	1A	3489	1/1	0.86	0.53	69,69,69,69	0
53	MG	1A	3257	1/1	0.86	0.29	40,40,40,40	0
53	MG	1A	3089	1/1	0.86	0.46	45,45,45,45	0
53	MG	2A	3450	1/1	0.86	0.35	103,103,103,103	0
53	MG	2a	1809	1/1	0.86	0.15	65,65,65,65	0
53	MG	1A	3602	1/1	0.86	0.28	58,58,58,58	0
53	MG	1A	3300	1/1	0.86	0.17	69,69,69,69	0
53	MG	1A	3001	1/1	0.86	0.39	57,57,57,57	0
53	MG	1A	3764	1/1	0.86	0.33	71,71,71,71	0
53	MG	2a	1751	1/1	0.86	0.19	109,109,109,109	0
53	MG	1A	3019	1/1	0.86	0.12	93,93,93,93	0
53	MG	2A	3417	1/1	0.86	0.35	81,81,81,81	0
53	MG	1a	1889	1/1	0.86	0.14	63,63,63,63	0
53	MG	1A	3701	1/1	0.86	0.20	45,45,45,45	0
53	MG	2A	3317	1/1	0.86	0.09	105,105,105,105	0
53	MG	1A	3006	1/1	0.86	0.28	59,59,59,59	0
53	MG	1a	1766	1/1	0.86	0.54	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	2D	306	1/1	0.86	0.43	59,59,59,59	0
53	MG	2A	3217	1/1	0.86	0.23	66,66,66,66	0
53	MG	1a	1850	1/1	0.86	0.22	73,73,73,73	0
53	MG	1A	3562	1/1	0.86	0.47	65,65,65,65	0
53	MG	1A	3109	1/1	0.86	0.17	50,50,50,50	0
53	MG	1A	3670	1/1	0.86	0.26	85,85,85,85	0
53	MG	1d	503	1/1	0.86	0.15	120,120,120,120	0
53	MG	2A	3122	1/1	0.86	0.27	83,83,83,83	0
53	MG	2A	3336	1/1	0.86	0.30	73,73,73,73	0
53	MG	1a	1843	1/1	0.86	0.62	208,208,208,208	0
53	MG	1A	3805	1/1	0.86	0.10	80,80,80,80	0
53	MG	1A	3774	1/1	0.86	0.34	63,63,63,63	0
53	MG	1A	3516	1/1	0.86	0.62	70,70,70,70	0
53	MG	1A	3050	1/1	0.86	0.22	59,59,59,59	0
53	MG	1a	1764	1/1	0.86	0.53	68,68,68,68	0
53	MG	1A	3538	1/1	0.86	0.74	61,61,61,61	0
53	MG	2A	3168	1/1	0.87	0.13	71,71,71,71	0
53	MG	1A	3675	1/1	0.87	0.27	35,35,35,35	0
53	MG	1A	3031	1/1	0.87	0.13	60,60,60,60	0
53	MG	2A	3195	1/1	0.87	1.04	65,65,65,65	0
53	MG	1l	101	1/1	0.87	0.17	40,40,40,40	0
53	MG	1A	3362	1/1	0.87	0.34	59,59,59,59	0
53	MG	1A	3718	1/1	0.87	0.27	112,112,112,112	0
53	MG	1A	3284	1/1	0.87	0.19	66,66,66,66	0
53	MG	1a	1730	1/1	0.87	0.08	81,81,81,81	0
53	MG	1A	3403	1/1	0.87	0.19	55,55,55,55	0
53	MG	2A	3494	1/1	0.87	0.36	79,79,79,79	0
53	MG	2A	3356	1/1	0.87	0.36	75,75,75,75	0
53	MG	2A	3225	1/1	0.87	0.17	58,58,58,58	0
53	MG	2a	1720	1/1	0.87	0.19	68,68,68,68	0
53	MG	1A	3614	1/1	0.87	0.23	68,68,68,68	0
53	MG	2a	1726	1/1	0.87	0.11	188,188,188,188	0
53	MG	1a	1814	1/1	0.87	0.17	84,84,84,84	0
53	MG	2A	3140	1/1	0.87	0.42	81,81,81,81	0
53	MG	1a	1886	1/1	0.87	0.67	83,83,83,83	0
53	MG	2A	3532	1/1	0.87	0.18	70,70,70,70	0
53	MG	1A	3584	1/1	0.87	0.18	55,55,55,55	0
53	MG	2G	8001	1/1	0.87	0.08	112,112,112,112	0
53	MG	1A	3753	1/1	0.87	0.36	63,63,63,63	0
53	MG	1A	3746	1/1	0.87	0.23	118,118,118,118	0
53	MG	2A	3533	1/1	0.87	0.41	55,55,55,55	0
53	MG	1A	3420	1/1	0.87	0.30	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	1a	1816	1/1	0.87	0.06	125,125,125,125	0
53	MG	2A	3400	1/1	0.87	0.34	81,81,81,81	0
53	MG	1A	3560	1/1	0.87	0.27	65,65,65,65	0
53	MG	1a	1825	1/1	0.87	0.50	98,98,98,98	0
53	MG	1A	3749	1/1	0.87	0.79	57,57,57,57	0
53	MG	2A	3138	1/1	0.87	0.52	79,79,79,79	0
53	MG	1F	307	1/1	0.87	0.55	87,87,87,87	0
53	MG	1A	3210	1/1	0.87	0.27	53,53,53,53	0
53	MG	2A	3167	1/1	0.87	0.21	87,87,87,87	0
53	MG	2a	1803	1/1	0.87	0.14	146,146,146,146	0
53	MG	2A	3310	1/1	0.87	0.36	70,70,70,70	0
53	MG	1A	3762	1/1	0.87	0.38	86,86,86,86	0
53	MG	2A	3502	1/1	0.87	0.20	84,84,84,84	0
53	MG	2A	3365	1/1	0.87	0.26	69,69,69,69	0
53	MG	1A	3128	1/1	0.87	0.71	87,87,87,87	0
53	MG	1A	3623	1/1	0.87	0.61	97,97,97,97	0
53	MG	2A	3250	1/1	0.87	0.28	104,104,104,104	0
53	MG	1A	3773	1/1	0.87	0.18	67,67,67,67	0
53	MG	1A	3363	1/1	0.87	0.22	67,67,67,67	0
53	MG	1A	3029	1/1	0.87	0.14	72,72,72,72	0
53	MG	1A	3022	1/1	0.87	0.32	76,76,76,76	0
53	MG	1A	3778	1/1	0.87	0.56	82,82,82,82	0
53	MG	1B	217	1/1	0.87	0.23	60,60,60,60	0
53	MG	1A	3393	1/1	0.87	0.61	62,62,62,62	0
53	MG	2a	1823	1/1	0.87	0.26	102,102,102,102	0
53	MG	1A	3212	1/1	0.87	0.29	51,51,51,51	0
53	MG	1A	3058	1/1	0.87	0.30	57,57,57,57	0
53	MG	2A	3223	1/1	0.87	0.33	56,56,56,56	0
53	MG	1A	3370	1/1	0.88	0.25	30,30,30,30	0
53	MG	1A	3285	1/1	0.88	0.20	27,27,27,27	0
53	MG	1A	3492	1/1	0.88	0.28	69,69,69,69	0
53	MG	1a	1742	1/1	0.88	0.24	117,117,117,117	0
53	MG	2A	3079	1/1	0.88	0.61	103,103,103,103	0
53	MG	1A	3663	1/1	0.88	0.32	54,54,54,54	0
53	MG	1A	3577	1/1	0.88	0.27	64,64,64,64	0
53	MG	2A	3535	1/1	0.88	0.16	84,84,84,84	0
53	MG	1A	3412	1/1	0.88	0.55	91,91,91,91	0
53	MG	1a	1751	1/1	0.88	0.39	105,105,105,105	0
53	MG	2A	3073	1/1	0.88	0.30	60,60,60,60	0
53	MG	2A	3160	1/1	0.88	0.30	93,93,93,93	0
53	MG	1A	3164	1/1	0.88	0.54	77,77,77,77	0
53	MG	2A	3335	1/1	0.88	0.20	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	1H	203	1/1	0.88	0.42	77,77,77,77	0
53	MG	1A	3696	1/1	0.88	0.39	45,45,45,45	0
53	MG	2A	3132	1/1	0.88	0.32	78,78,78,78	0
53	MG	1a	1732	1/1	0.88	0.11	110,110,110,110	0
53	MG	1A	3641	1/1	0.88	0.08	57,57,57,57	0
56	FSD	2A	3553	44/44	0.88	0.26	61,91,113,126	0
53	MG	1a	1885	1/1	0.88	0.17	86,86,86,86	0
53	MG	1A	3759	1/1	0.88	0.31	79,79,79,79	0
53	MG	2a	1752	1/1	0.88	0.49	127,127,127,127	0
53	MG	2A	3002	1/1	0.88	0.12	74,74,74,74	0
53	MG	2A	3476	1/1	0.88	0.61	132,132,132,132	0
53	MG	1A	3537	1/1	0.88	0.34	78,78,78,78	0
53	MG	2A	3506	1/1	0.88	0.31	65,65,65,65	0
53	MG	2A	3422	1/1	0.88	0.35	73,73,73,73	0
53	MG	2A	3531	1/1	0.88	0.26	94,94,94,94	0
53	MG	1a	1880	1/1	0.88	0.20	67,67,67,67	0
53	MG	2A	3346	1/1	0.88	0.83	76,76,76,76	0
53	MG	1a	1791	1/1	0.88	0.26	72,72,72,72	0
53	MG	2A	3375	1/1	0.88	0.79	100,100,100,100	0
53	MG	2A	3364	1/1	0.88	0.42	69,69,69,69	0
53	MG	1a	1794	1/1	0.88	0.38	73,73,73,73	0
53	MG	2A	3071	1/1	0.88	0.28	70,70,70,70	0
53	MG	1a	1763	1/1	0.88	0.29	101,101,101,101	0
53	MG	1A	3457	1/1	0.88	1.72	65,65,65,65	0
53	MG	1A	3153	1/1	0.88	0.37	107,107,107,107	0
53	MG	1A	3288	1/1	0.88	0.42	72,72,72,72	0
53	MG	1A	3352	1/1	0.88	0.25	52,52,52,52	0
53	MG	1A	3205	1/1	0.88	0.17	65,65,65,65	0
53	MG	2A	3406	1/1	0.88	0.14	83,83,83,83	0
53	MG	1A	3788	1/1	0.88	0.26	52,52,52,52	0
53	MG	1a	1835	1/1	0.88	0.44	131,131,131,131	0
53	MG	1B	204	1/1	0.88	0.40	68,68,68,68	0
53	MG	2A	3528	1/1	0.88	0.33	85,85,85,85	0
53	MG	2A	3244	1/1	0.88	0.19	109,109,109,109	0
53	MG	2A	3560	1/1	0.88	0.41	96,96,96,96	0
53	MG	2A	3044	1/1	0.88	0.24	79,79,79,79	0
53	MG	1A	3369	1/1	0.88	0.34	22,22,22,22	0
53	MG	2a	1800	1/1	0.88	0.25	79,79,79,79	0
53	MG	2A	3358	1/1	0.88	0.32	78,78,78,78	0
53	MG	1A	3095	1/1	0.88	0.36	53,53,53,53	0
53	MG	1A	3566	1/1	0.88	0.41	62,62,62,62	0
53	MG	1E	307	1/1	0.88	0.29	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	1a	1827	1/1	0.88	0.44	76,76,76,76	0
53	MG	1a	1879	1/1	0.88	0.57	72,72,72,72	0
53	MG	1a	1884	1/1	0.88	0.12	104,104,104,104	0
53	MG	2A	3453	1/1	0.88	0.25	96,96,96,96	0
53	MG	2a	1764	1/1	0.88	0.58	139,139,139,139	0
53	MG	2A	3227	1/1	0.88	0.29	61,61,61,61	0
53	MG	1a	1832	1/1	0.88	0.52	65,65,65,65	0
53	MG	2A	3477	1/1	0.88	0.45	115,115,115,115	0
53	MG	2a	1807	1/1	0.88	0.30	68,68,68,68	0
53	MG	2a	1810	1/1	0.88	0.39	58,58,58,58	0
53	MG	1A	3667	1/1	0.88	0.56	40,40,40,40	0
53	MG	2D	302	1/1	0.88	0.23	86,86,86,86	0
53	MG	1A	3459	1/1	0.88	0.30	53,53,53,53	0
53	MG	2A	3186	1/1	0.88	0.34	105,105,105,105	0
53	MG	19	103	1/1	0.88	0.55	86,86,86,86	0
53	MG	2A	3074	1/1	0.88	0.14	101,101,101,101	0
53	MG	1A	3821	1/1	0.88	0.82	86,86,86,86	0
53	MG	1a	1901	1/1	0.89	0.10	91,91,91,91	0
53	MG	1A	3604	1/1	0.89	0.36	81,81,81,81	0
53	MG	1A	3059	1/1	0.89	0.51	67,67,67,67	0
53	MG	1a	1805	1/1	0.89	0.09	86,86,86,86	0
53	MG	2A	3288	1/1	0.89	0.28	83,83,83,83	0
53	MG	1A	3568	1/1	0.89	0.47	44,44,44,44	0
53	MG	2A	3339	1/1	0.89	0.15	80,80,80,80	0
53	MG	1A	3438	1/1	0.89	0.28	66,66,66,66	0
53	MG	1A	3722	1/1	0.89	0.20	89,89,89,89	0
53	MG	1A	3040	1/1	0.89	0.84	61,61,61,61	0
53	MG	1A	3134	1/1	0.89	0.27	73,73,73,73	0
53	MG	2a	1784	1/1	0.89	0.18	68,68,68,68	0
53	MG	1a	1899	1/1	0.89	0.24	102,102,102,102	0
53	MG	2A	3279	1/1	0.89	0.32	92,92,92,92	0
53	MG	1a	1834	1/1	0.89	0.29	102,102,102,102	0
53	MG	2A	3363	1/1	0.89	0.56	126,126,126,126	0
53	MG	1A	3238	1/1	0.89	0.27	89,89,89,89	0
53	MG	2A	3309	1/1	0.89	0.41	82,82,82,82	0
53	MG	1A	3544	1/1	0.89	0.21	36,36,36,36	0
53	MG	1A	3264	1/1	0.89	0.32	46,46,46,46	0
53	MG	1A	3144	1/1	0.89	0.18	92,92,92,92	0
53	MG	1B	205	1/1	0.89	0.12	76,76,76,76	0
53	MG	1A	3279	1/1	0.89	0.22	53,53,53,53	0
53	MG	1A	3628	1/1	0.89	0.29	59,59,59,59	0
53	MG	1A	3069	1/1	0.89	0.44	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	1A	3131	1/1	0.89	0.31	89,89,89,89	0
53	MG	1A	3322	1/1	0.89	0.11	80,80,80,80	0
53	MG	1D	304	1/1	0.89	0.21	81,81,81,81	0
53	MG	1A	3792	1/1	0.89	0.72	61,61,61,61	0
53	MG	1A	3265	1/1	0.89	0.34	41,41,41,41	0
53	MG	1A	3570	1/1	0.89	0.26	40,40,40,40	0
53	MG	10	106	1/1	0.89	0.21	72,72,72,72	0
53	MG	1E	302	1/1	0.89	0.66	42,42,42,42	0
53	MG	1A	3065	1/1	0.89	0.25	58,58,58,58	0
53	MG	1a	1779	1/1	0.89	0.21	100,100,100,100	0
53	MG	2A	3413	1/1	0.89	0.76	93,93,93,93	0
53	MG	1a	1705	1/1	0.89	0.18	82,82,82,82	0
53	MG	1A	3338	1/1	0.89	0.37	74,74,74,74	0
53	MG	2A	3206	1/1	0.89	0.12	80,80,80,80	0
53	MG	2A	3042	1/1	0.89	0.38	83,83,83,83	0
53	MG	1A	3550	1/1	0.89	0.27	49,49,49,49	0
53	MG	2A	3405	1/1	0.89	0.33	77,77,77,77	0
53	MG	2A	3020	1/1	0.89	0.10	77,77,77,77	0
53	MG	2A	3323	1/1	0.89	0.41	101,101,101,101	0
53	MG	1A	3840	1/1	0.89	1.03	41,41,41,41	0
53	MG	1A	3425	1/1	0.89	0.21	79,79,79,79	0
56	FSD	1A	3801	44/44	0.89	0.28	24,64,94,111	0
53	MG	1A	3728	1/1	0.89	0.62	69,69,69,69	0
53	MG	1A	3045	1/1	0.89	0.59	70,70,70,70	0
53	MG	2A	3416	1/1	0.89	0.18	71,71,71,71	0
53	MG	1A	3062	1/1	0.89	0.26	58,58,58,58	0
53	MG	1A	3209	1/1	0.89	0.44	81,81,81,81	0
53	MG	2A	3171	1/1	0.89	0.22	73,73,73,73	0
53	MG	1a	1860	1/1	0.89	0.29	92,92,92,92	0
53	MG	1l	3001	1/1	0.89	0.25	78,78,78,78	0
53	MG	2A	3321	1/1	0.89	0.80	67,67,67,67	0
53	MG	1A	3435	1/1	0.89	0.34	66,66,66,66	0
53	MG	1A	3133	1/1	0.89	0.27	65,65,65,65	0
53	MG	2A	3137	1/1	0.89	0.41	66,66,66,66	0
53	MG	2A	3404	1/1	0.89	0.33	83,83,83,83	0
53	MG	1A	3563	1/1	0.89	0.43	56,56,56,56	0
53	MG	2a	1790	1/1	0.89	0.26	96,96,96,96	0
53	MG	2A	3503	1/1	0.89	0.29	76,76,76,76	0
53	MG	2A	3496	1/1	0.89	0.20	77,77,77,77	0
53	MG	1A	3232	1/1	0.89	0.13	63,63,63,63	0
53	MG	2A	3235	1/1	0.89	0.19	54,54,54,54	0
53	MG	1A	3825	1/1	0.89	0.19	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	2A	3165	1/1	0.89	0.23	73,73,73,73	0
53	MG	1A	3776	1/1	0.89	0.80	48,48,48,48	0
53	MG	1A	3064	1/1	0.89	0.43	57,57,57,57	0
53	MG	1A	3745	1/1	0.89	0.41	88,88,88,88	0
53	MG	1A	3401	1/1	0.89	0.52	54,54,54,54	0
53	MG	2A	3065	1/1	0.89	0.20	76,76,76,76	0
53	MG	1Y	502	1/1	0.89	0.19	100,100,100,100	0
53	MG	1A	3443	1/1	0.89	0.46	90,90,90,90	0
53	MG	1a	1875	1/1	0.89	0.29	58,58,58,58	0
53	MG	1A	3408	1/1	0.89	0.29	85,85,85,85	0
53	MG	2A	3483	1/1	0.89	0.15	99,99,99,99	0
53	MG	1A	3082	1/1	0.89	0.31	53,53,53,53	0
53	MG	1a	1828	1/1	0.89	0.86	123,123,123,123	0
53	MG	2A	3307	1/1	0.89	0.34	107,107,107,107	0
53	MG	2A	3423	1/1	0.89	0.31	96,96,96,96	0
53	MG	2A	3203	1/1	0.89	0.44	74,74,74,74	0
53	MG	1a	1806	1/1	0.89	0.11	119,119,119,119	0
53	MG	2D	303	1/1	0.89	0.40	77,77,77,77	0
53	MG	1A	3385	1/1	0.89	0.22	70,70,70,70	0
53	MG	1A	3052	1/1	0.89	0.37	61,61,61,61	0
53	MG	1A	3098	1/1	0.89	0.29	45,45,45,45	0
53	MG	2A	3136	1/1	0.89	0.21	75,75,75,75	0
53	MG	1A	3303	1/1	0.89	0.20	95,95,95,95	0
53	MG	2A	3033	1/1	0.89	0.07	129,129,129,129	0
53	MG	1A	3490	1/1	0.89	0.66	85,85,85,85	0
53	MG	1a	1895	1/1	0.89	0.83	66,66,66,66	0
53	MG	1A	3480	1/1	0.89	0.41	92,92,92,92	0
53	MG	1A	3216	1/1	0.90	0.31	48,48,48,48	0
53	MG	1a	1786	1/1	0.90	0.12	73,73,73,73	0
53	MG	2a	1729	1/1	0.90	0.18	75,75,75,75	0
53	MG	1A	3830	1/1	0.90	0.47	62,62,62,62	0
53	MG	1A	3786	1/1	0.90	0.80	63,63,63,63	0
53	MG	1A	3394	1/1	0.90	0.50	92,92,92,92	0
53	MG	2A	3286	1/1	0.90	0.70	79,79,79,79	0
53	MG	1A	3382	1/1	0.90	0.14	71,71,71,71	0
53	MG	1a	1804	1/1	0.90	0.14	85,85,85,85	0
53	MG	2A	3150	1/1	0.90	0.42	79,79,79,79	0
53	MG	1A	3608	1/1	0.90	0.23	70,70,70,70	0
53	MG	2a	1811	1/1	0.90	0.38	73,73,73,73	0
53	MG	1A	3442	1/1	0.90	0.26	84,84,84,84	0
53	MG	1a	1702	1/1	0.90	0.29	81,81,81,81	0
53	MG	2A	3369	1/1	0.90	0.14	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	2A	3108	1/1	0.90	0.28	81,81,81,81	0
53	MG	1A	3415	1/1	0.90	0.44	91,91,91,91	0
53	MG	1A	3258	1/1	0.90	0.32	59,59,59,59	0
53	MG	1A	3003	1/1	0.90	0.16	50,50,50,50	0
53	MG	1a	1743	1/1	0.90	0.74	74,74,74,74	0
53	MG	2A	3320	1/1	0.90	0.32	80,80,80,80	0
53	MG	1A	3658	1/1	0.90	0.27	40,40,40,40	0
53	MG	2A	3095	1/1	0.90	0.17	91,91,91,91	0
53	MG	1D	314	1/1	0.90	0.40	72,72,72,72	0
53	MG	2A	3213	1/1	0.90	0.37	71,71,71,71	0
53	MG	1b	3001	1/1	0.90	0.09	132,132,132,132	0
53	MG	1A	3139	1/1	0.90	0.13	37,37,37,37	0
53	MG	1A	3523	1/1	0.90	0.06	59,59,59,59	0
53	MG	1A	3418	1/1	0.90	0.25	64,64,64,64	0
53	MG	1A	3449	1/1	0.90	0.41	68,68,68,68	0
53	MG	2A	3292	1/1	0.90	0.30	78,78,78,78	0
53	MG	1A	3655	1/1	0.90	0.28	62,62,62,62	0
53	MG	2A	3338	1/1	0.90	0.17	86,86,86,86	0
53	MG	1F	302	1/1	0.90	0.31	72,72,72,72	0
53	MG	2A	3221	1/1	0.90	0.18	65,65,65,65	0
53	MG	1F	305	1/1	0.90	0.62	39,39,39,39	0
53	MG	2A	3207	1/1	0.90	0.62	75,75,75,75	0
53	MG	1B	211	1/1	0.90	0.29	68,68,68,68	0
53	MG	1A	3358	1/1	0.90	0.18	75,75,75,75	0
53	MG	1a	1738	1/1	0.90	0.55	177,177,177,177	0
53	MG	2A	3504	1/1	0.90	0.22	58,58,58,58	0
53	MG	1B	212	1/1	0.90	0.24	55,55,55,55	0
53	MG	1A	3105	1/1	0.90	0.42	69,69,69,69	0
53	MG	2A	3172	1/1	0.90	0.24	45,45,45,45	0
53	MG	1A	3225	1/1	0.90	0.69	44,44,44,44	0
53	MG	1A	3685	1/1	0.90	0.27	62,62,62,62	0
53	MG	2A	3324	1/1	0.90	0.25	78,78,78,78	0
53	MG	15	102	1/1	0.90	0.28	50,50,50,50	0
53	MG	1A	3320	1/1	0.90	0.26	73,73,73,73	0
53	MG	1A	3515	1/1	0.90	0.20	61,61,61,61	0
53	MG	1A	3180	1/1	0.90	0.22	71,71,71,71	0
53	MG	1A	3405	1/1	0.90	0.27	73,73,73,73	0
53	MG	2A	3384	1/1	0.90	0.34	97,97,97,97	0
53	MG	1A	3441	1/1	0.90	0.16	63,63,63,63	0
53	MG	1A	3193	1/1	0.90	0.25	59,59,59,59	0
53	MG	1A	3218	1/1	0.90	0.10	71,71,71,71	0
53	MG	2a	1841	1/1	0.90	0.53	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	2A	3242	1/1	0.90	0.42	60,60,60,60	0
53	MG	1D	315	1/1	0.90	0.66	63,63,63,63	0
55	MPD	1A	3800	8/8	0.90	0.27	67,80,94,98	0
53	MG	1a	1807	1/1	0.90	0.24	69,69,69,69	0
53	MG	2A	3517	1/1	0.90	0.21	86,86,86,86	0
53	MG	1A	3747	1/1	0.90	0.14	96,96,96,96	0
53	MG	1A	3613	1/1	0.90	0.60	60,60,60,60	0
53	MG	2A	3152	1/1	0.90	0.73	72,72,72,72	0
55	MPD	1a	1900	8/8	0.90	0.38	80,100,105,111	0
57	ZN	29	501	1/1	0.90	0.15	136,136,136,136	0
53	MG	1A	3816	1/1	0.90	0.54	31,31,31,31	0
53	MG	2A	3441	1/1	0.90	0.36	57,57,57,57	0
53	MG	2A	3380	1/1	0.90	0.24	65,65,65,65	0
53	MG	1a	1870	1/1	0.90	0.15	101,101,101,101	0
53	MG	1A	3106	1/1	0.90	0.14	84,84,84,84	0
53	MG	2a	1828	1/1	0.90	0.66	103,103,103,103	0
53	MG	1A	3015	1/1	0.90	0.33	39,39,39,39	0
53	MG	2a	1838	1/1	0.90	0.27	69,69,69,69	0
53	MG	2A	3557	1/1	0.90	0.24	58,58,58,58	0
53	MG	2A	3398	1/1	0.90	0.22	89,89,89,89	0
53	MG	1A	3829	1/1	0.90	0.25	64,64,64,64	0
53	MG	2A	3214	1/1	0.90	0.28	66,66,66,66	0
53	MG	2a	1821	1/1	0.90	0.12	115,115,115,115	0
53	MG	1a	1871	1/1	0.90	0.39	74,74,74,74	0
53	MG	2A	3036	1/1	0.90	0.34	76,76,76,76	0
53	MG	2l	101	1/1	0.90	0.98	70,70,70,70	0
53	MG	2A	3046	1/1	0.90	0.24	68,68,68,68	0
53	MG	2a	1719	1/1	0.90	0.17	48,48,48,48	0
53	MG	2A	3179	1/1	0.90	0.20	59,59,59,59	0
53	MG	1A	3820	1/1	0.90	0.18	39,39,39,39	0
53	MG	1a	1701	1/1	0.91	0.14	71,71,71,71	0
53	MG	1A	3396	1/1	0.91	0.19	80,80,80,80	0
53	MG	1A	3626	1/1	0.91	0.28	57,57,57,57	0
53	MG	1Z	8002	1/1	0.91	0.18	55,55,55,55	0
53	MG	18	103	1/1	0.91	0.23	73,73,73,73	0
53	MG	28	8003	1/1	0.91	0.33	87,87,87,87	0
53	MG	18	101	1/1	0.91	0.40	69,69,69,69	0
53	MG	1A	3315	1/1	0.91	0.33	64,64,64,64	0
53	MG	1A	3308	1/1	0.91	0.79	80,80,80,80	0
53	MG	2A	3267	1/1	0.91	0.50	56,56,56,56	0
53	MG	1A	3671	1/1	0.91	0.34	58,58,58,58	0
53	MG	2A	3297	1/1	0.91	0.21	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	1A	3476	1/1	0.91	0.29	62,62,62,62	0
53	MG	1A	3101	1/1	0.91	0.09	54,54,54,54	0
53	MG	1A	3713	1/1	0.91	0.18	68,68,68,68	0
53	MG	1a	1824	1/1	0.91	0.15	76,76,76,76	0
53	MG	2A	3184	1/1	0.91	0.41	67,67,67,67	0
53	MG	1A	3798	1/1	0.91	0.28	69,69,69,69	0
53	MG	2a	1775	1/1	0.91	0.51	90,90,90,90	0
53	MG	1A	3398	1/1	0.91	0.40	71,71,71,71	0
53	MG	2A	3200	1/1	0.91	0.27	59,59,59,59	0
53	MG	1A	3674	1/1	0.91	0.16	45,45,45,45	0
53	MG	1A	3760	1/1	0.91	0.32	81,81,81,81	0
53	MG	1a	1787	1/1	0.91	0.83	118,118,118,118	0
53	MG	2A	3022	1/1	0.91	0.59	59,59,59,59	0
53	MG	1N	204	1/1	0.91	0.24	37,37,37,37	0
53	MG	1A	3507	1/1	0.91	0.17	118,118,118,118	0
53	MG	1A	3818	1/1	0.91	0.40	76,76,76,76	0
53	MG	1A	3462	1/1	0.91	0.21	55,55,55,55	0
53	MG	1a	1703	1/1	0.91	0.12	97,97,97,97	0
53	MG	1A	3351	1/1	0.91	0.13	52,52,52,52	0
53	MG	2A	3127	1/1	0.91	0.10	67,67,67,67	0
53	MG	1A	3607	1/1	0.91	0.39	71,71,71,71	0
53	MG	1A	3698	1/1	0.91	0.13	78,78,78,78	0
53	MG	1A	3699	1/1	0.91	0.41	71,71,71,71	0
53	MG	1A	3427	1/1	0.91	0.37	64,64,64,64	0
53	MG	2A	3283	1/1	0.91	0.24	56,56,56,56	0
53	MG	1A	3669	1/1	0.91	0.28	69,69,69,69	0
53	MG	1T	8001	1/1	0.91	0.16	95,95,95,95	0
53	MG	1A	3734	1/1	0.91	0.74	83,83,83,83	0
53	MG	2A	3100	1/1	0.91	0.13	79,79,79,79	0
53	MG	2A	3246	1/1	0.91	0.22	65,65,65,65	0
53	MG	2A	3302	1/1	0.91	0.17	70,70,70,70	0
53	MG	1A	3360	1/1	0.91	0.20	67,67,67,67	0
53	MG	1A	3575	1/1	0.91	0.31	73,73,73,73	0
53	MG	1a	1841	1/1	0.91	0.40	69,69,69,69	0
53	MG	1A	3233	1/1	0.91	0.28	35,35,35,35	0
53	MG	2A	3282	1/1	0.91	0.17	110,110,110,110	0
53	MG	2A	3401	1/1	0.91	0.29	61,61,61,61	0
53	MG	1A	3571	1/1	0.91	0.23	63,63,63,63	0
53	MG	1A	3171	1/1	0.91	0.23	73,73,73,73	0
53	MG	2A	3555	1/1	0.91	0.20	225,225,225,225	0
53	MG	1A	3832	1/1	0.91	0.26	41,41,41,41	0
53	MG	2A	3055	1/1	0.91	0.28	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	1A	3498	1/1	0.91	0.44	69,69,69,69	0
53	MG	1A	3332	1/1	0.91	0.23	50,50,50,50	0
53	MG	2a	1805	1/1	0.91	0.74	105,105,105,105	0
53	MG	2A	3361	1/1	0.91	0.33	95,95,95,95	0
54	ARG	1B	223	12/12	0.91	0.37	25,48,89,97	0
53	MG	2A	3086	1/1	0.91	0.25	106,106,106,106	0
53	MG	1A	3406	1/1	0.91	0.32	78,78,78,78	0
53	MG	2A	3247	1/1	0.91	0.54	72,72,72,72	0
53	MG	1A	3767	1/1	0.91	0.21	55,55,55,55	0
53	MG	2A	3394	1/1	0.91	0.30	105,105,105,105	0
53	MG	2A	3161	1/1	0.91	0.23	97,97,97,97	0
53	MG	2A	3155	1/1	0.91	0.47	104,104,104,104	0
53	MG	1a	1762	1/1	0.91	0.20	63,63,63,63	0
53	MG	1A	3423	1/1	0.91	0.74	62,62,62,62	0
53	MG	2a	1736	1/1	0.91	0.17	125,125,125,125	0
53	MG	2A	3269	1/1	0.91	0.17	70,70,70,70	0
53	MG	1A	3679	1/1	0.91	0.54	68,68,68,68	0
53	MG	2Z	301	1/1	0.91	0.28	99,99,99,99	0
53	MG	2A	3377	1/1	0.91	0.18	82,82,82,82	0
53	MG	2A	3360	1/1	0.91	0.16	53,53,53,53	0
53	MG	1A	3072	1/1	0.91	0.33	69,69,69,69	0
53	MG	1A	3290	1/1	0.91	0.26	51,51,51,51	0
53	MG	1A	3329	1/1	0.91	0.28	64,64,64,64	0
53	MG	1A	3662	1/1	0.91	0.41	72,72,72,72	0
53	MG	1A	3025	1/1	0.91	0.65	79,79,79,79	0
53	MG	1A	3477	1/1	0.91	0.19	57,57,57,57	0
53	MG	2A	3395	1/1	0.91	0.09	84,84,84,84	0
53	MG	2A	3326	1/1	0.91	0.15	105,105,105,105	0
53	MG	1A	3726	1/1	0.91	0.12	82,82,82,82	0
53	MG	2A	3191	1/1	0.91	0.69	75,75,75,75	0
53	MG	2A	3004	1/1	0.91	0.20	72,72,72,72	0
53	MG	2A	3228	1/1	0.91	0.32	59,59,59,59	0
53	MG	2A	3515	1/1	0.91	0.16	76,76,76,76	0
53	MG	1A	3366	1/1	0.91	0.32	84,84,84,84	0
57	ZN	2Y	501	1/1	0.91	0.11	143,143,143,143	0
53	MG	1A	3271	1/1	0.91	0.29	81,81,81,81	0
53	MG	2A	3204	1/1	0.91	0.16	81,81,81,81	0
53	MG	1a	1765	1/1	0.91	0.19	83,83,83,83	0
53	MG	2Y	502	1/1	0.91	0.13	90,90,90,90	0
53	MG	2A	3355	1/1	0.91	0.46	69,69,69,69	0
53	MG	1A	3810	1/1	0.91	0.28	55,55,55,55	0
53	MG	2A	3319	1/1	0.92	0.24	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	2a	1802	1/1	0.92	0.33	86,86,86,86	0
53	MG	2A	3498	1/1	0.92	0.40	59,59,59,59	0
53	MG	2P	203	1/1	0.92	0.12	81,81,81,81	0
53	MG	1A	3790	1/1	0.92	0.13	38,38,38,38	0
53	MG	2A	3463	1/1	0.92	0.32	68,68,68,68	0
53	MG	1A	3179	1/1	0.92	0.72	62,62,62,62	0
53	MG	1A	3350	1/1	0.92	0.20	52,52,52,52	0
53	MG	2a	1735	1/1	0.92	0.11	122,122,122,122	0
53	MG	2A	3218	1/1	0.92	0.21	76,76,76,76	0
53	MG	2A	3428	1/1	0.92	0.31	66,66,66,66	0
53	MG	1A	3646	1/1	0.92	0.15	83,83,83,83	0
53	MG	2A	3201	1/1	0.92	0.32	76,76,76,76	0
53	MG	1A	3682	1/1	0.92	0.21	72,72,72,72	0
53	MG	1A	3483	1/1	0.92	0.67	47,47,47,47	0
53	MG	1a	1799	1/1	0.92	0.17	63,63,63,63	0
53	MG	1a	1903	1/1	0.92	0.06	81,81,81,81	0
53	MG	1A	3680	1/1	0.92	0.19	28,28,28,28	0
53	MG	2A	3226	1/1	0.92	0.14	80,80,80,80	0
53	MG	2A	3270	1/1	0.92	0.20	89,89,89,89	0
53	MG	1A	3684	1/1	0.92	0.29	65,65,65,65	0
53	MG	1A	3356	1/1	0.92	0.44	68,68,68,68	0
53	MG	1A	3691	1/1	0.92	0.15	70,70,70,70	0
53	MG	2T	3001	1/1	0.92	0.22	95,95,95,95	0
53	MG	1A	3008	1/1	0.92	0.28	57,57,57,57	0
53	MG	2A	3144	1/1	0.92	0.21	64,64,64,64	0
53	MG	1A	3690	1/1	0.92	0.14	40,40,40,40	0
53	MG	1A	3155	1/1	0.92	0.36	67,67,67,67	0
53	MG	1a	1803	1/1	0.92	0.23	81,81,81,81	0
53	MG	1A	3444	1/1	0.92	0.28	66,66,66,66	0
53	MG	2A	3316	1/1	0.92	0.51	74,74,74,74	0
53	MG	1A	3136	1/1	0.92	0.53	93,93,93,93	0
53	MG	2A	3329	1/1	0.92	0.25	65,65,65,65	0
53	MG	2A	3352	1/1	0.92	0.32	86,86,86,86	0
53	MG	1A	3227	1/1	0.92	0.24	41,41,41,41	0
53	MG	1A	3104	1/1	0.92	0.72	69,69,69,69	0
53	MG	1A	3761	1/1	0.92	0.47	52,52,52,52	0
53	MG	1a	1887	1/1	0.92	0.70	60,60,60,60	0
53	MG	1A	3011	1/1	0.92	0.44	78,78,78,78	0
53	MG	2A	3041	1/1	0.92	0.22	66,66,66,66	0
53	MG	2A	3429	1/1	0.92	0.31	78,78,78,78	0
53	MG	1A	3333	1/1	0.92	0.17	91,91,91,91	0
53	MG	2A	3253	1/1	0.92	0.16	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	2a	1739	1/1	0.92	0.12	164,164,164,164	0
53	MG	1l	3002	1/1	0.92	0.10	70,70,70,70	0
53	MG	1A	3211	1/1	0.92	0.25	76,76,76,76	0
53	MG	1A	3317	1/1	0.92	0.15	57,57,57,57	0
53	MG	2A	3190	1/1	0.92	0.24	74,74,74,74	0
53	MG	1A	3041	1/1	0.92	0.30	72,72,72,72	0
53	MG	2A	3337	1/1	0.92	0.10	79,79,79,79	0
53	MG	1A	3757	1/1	0.92	0.34	87,87,87,87	0
53	MG	2A	3530	1/1	0.92	0.28	69,69,69,69	0
53	MG	2a	1829	1/1	0.92	0.25	99,99,99,99	0
53	MG	1A	3535	1/1	0.92	0.28	74,74,74,74	0
53	MG	2A	3308	1/1	0.92	0.94	92,92,92,92	0
53	MG	1A	3723	1/1	0.92	0.24	63,63,63,63	0
53	MG	1E	303	1/1	0.92	0.31	82,82,82,82	0
53	MG	1A	3783	1/1	0.92	0.27	65,65,65,65	0
53	MG	1A	3313	1/1	0.92	0.45	45,45,45,45	0
53	MG	1A	3237	1/1	0.92	0.29	65,65,65,65	0
53	MG	1a	1883	1/1	0.92	0.18	65,65,65,65	0
53	MG	1A	3775	1/1	0.92	0.24	54,54,54,54	0
53	MG	1a	1809	1/1	0.92	0.17	94,94,94,94	0
53	MG	1A	3725	1/1	0.92	0.19	63,63,63,63	0
53	MG	2A	3412	1/1	0.92	0.43	72,72,72,72	0
53	MG	2A	3421	1/1	0.92	0.23	112,112,112,112	0
53	MG	1A	3834	1/1	0.92	0.14	57,57,57,57	0
53	MG	1A	3195	1/1	0.92	0.19	52,52,52,52	0
53	MG	2a	1817	1/1	0.92	0.48	81,81,81,81	0
53	MG	1A	3756	1/1	0.92	0.38	56,56,56,56	0
53	MG	1A	3660	1/1	0.92	0.34	54,54,54,54	0
53	MG	1A	3166	1/1	0.92	0.22	154,154,154,154	0
53	MG	2A	3019	1/1	0.92	0.24	77,77,77,77	0
53	MG	1A	3458	1/1	0.92	1.35	78,78,78,78	0
53	MG	2A	3314	1/1	0.92	0.09	80,80,80,80	0
53	MG	2A	3093	1/1	0.92	0.14	93,93,93,93	0
53	MG	1A	3326	1/1	0.92	0.16	73,73,73,73	0
53	MG	1A	3580	1/1	0.92	0.16	60,60,60,60	0
53	MG	1A	3652	1/1	0.92	0.25	71,71,71,71	0
53	MG	1a	1712	1/1	0.92	0.08	123,123,123,123	0
53	MG	1A	3307	1/1	0.92	0.40	66,66,66,66	0
53	MG	1A	3327	1/1	0.92	0.20	84,84,84,84	0
53	MG	1A	3141	1/1	0.92	0.26	64,64,64,64	0
53	MG	1A	3738	1/1	0.92	0.15	40,40,40,40	0
53	MG	1U	201	1/1	0.92	0.28	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	1B	215	1/1	0.92	0.21	45,45,45,45	0
53	MG	1S	201	1/1	0.92	0.74	84,84,84,84	0
53	MG	1A	3620	1/1	0.92	0.36	75,75,75,75	0
53	MG	1A	3453	1/1	0.92	0.26	66,66,66,66	0
55	MPD	18	104	8/8	0.92	0.30	32,49,55,65	0
53	MG	2a	1763	1/1	0.92	0.20	83,83,83,83	0
53	MG	1A	3379	1/1	0.92	0.32	53,53,53,53	0
53	MG	1A	3386	1/1	0.92	0.23	40,40,40,40	0
53	MG	2A	3208	1/1	0.92	0.25	48,48,48,48	0
53	MG	1a	1777	1/1	0.92	0.22	164,164,164,164	0
53	MG	2a	1747	1/1	0.92	0.22	88,88,88,88	0
53	MG	2A	3490	1/1	0.92	0.41	62,62,62,62	0
53	MG	2A	3237	1/1	0.92	0.28	54,54,54,54	0
53	MG	2A	3374	1/1	0.92	0.27	59,59,59,59	0
53	MG	1A	3592	1/1	0.92	0.26	74,74,74,74	0
53	MG	1A	3797	1/1	0.92	0.29	60,60,60,60	0
53	MG	1a	1813	1/1	0.92	0.34	74,74,74,74	0
53	MG	1A	3152	1/1	0.92	0.28	87,87,87,87	0
53	MG	2A	3245	1/1	0.92	0.12	68,68,68,68	0
53	MG	1A	3092	1/1	0.93	0.51	51,51,51,51	0
53	MG	1A	3430	1/1	0.93	0.22	53,53,53,53	0
53	MG	2A	3027	1/1	0.93	0.28	95,95,95,95	0
53	MG	1A	3564	1/1	0.93	0.28	52,52,52,52	0
53	MG	1A	3375	1/1	0.93	0.48	57,57,57,57	0
53	MG	1a	1822	1/1	0.93	0.10	60,60,60,60	0
53	MG	2D	305	1/1	0.93	0.31	115,115,115,115	0
53	MG	1A	3223	1/1	0.93	0.54	44,44,44,44	0
53	MG	2A	3512	1/1	0.93	0.14	79,79,79,79	0
53	MG	1A	3275	1/1	0.93	0.31	42,42,42,42	0
53	MG	1A	3085	1/1	0.93	0.18	64,64,64,64	0
53	MG	1P	203	1/1	0.93	0.19	59,59,59,59	0
53	MG	1A	3021	1/1	0.93	0.48	75,75,75,75	0
53	MG	1A	3510	1/1	0.93	0.33	74,74,74,74	0
53	MG	2A	3432	1/1	0.93	0.33	80,80,80,80	0
53	MG	2A	3445	1/1	0.93	0.36	83,83,83,83	0
53	MG	1G	8002	1/1	0.93	0.21	92,92,92,92	0
53	MG	1A	3543	1/1	0.93	0.25	56,56,56,56	0
53	MG	2A	3170	1/1	0.93	0.25	70,70,70,70	0
53	MG	1A	3053	1/1	0.93	0.26	72,72,72,72	0
53	MG	1A	3206	1/1	0.93	0.17	64,64,64,64	0
53	MG	2A	3467	1/1	0.93	0.16	79,79,79,79	0
53	MG	1A	3532	1/1	0.93	0.22	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	1A	3380	1/1	0.93	0.27	52,52,52,52	0
53	MG	2A	3403	1/1	0.93	0.20	102,102,102,102	0
53	MG	1A	3278	1/1	0.93	0.20	64,64,64,64	0
53	MG	2A	3300	1/1	0.93	0.13	51,51,51,51	0
53	MG	1A	3252	1/1	0.93	0.18	48,48,48,48	0
53	MG	2A	3275	1/1	0.93	0.40	81,81,81,81	0
53	MG	1A	3837	1/1	0.93	0.51	74,74,74,74	0
53	MG	2A	3564	1/1	0.93	0.50	82,82,82,82	0
53	MG	1A	3172	1/1	0.93	0.18	49,49,49,49	0
53	MG	2A	3458	1/1	0.93	0.18	73,73,73,73	0
53	MG	1A	3341	1/1	0.93	0.32	41,41,41,41	0
53	MG	1A	3609	1/1	0.93	0.21	51,51,51,51	0
53	MG	2A	3472	1/1	0.93	0.42	87,87,87,87	0
53	MG	1A	3730	1/1	0.93	0.50	84,84,84,84	0
53	MG	2A	3488	1/1	0.93	0.21	56,56,56,56	0
53	MG	1A	3013	1/1	0.93	0.16	43,43,43,43	0
53	MG	2A	3254	1/1	0.93	0.49	115,115,115,115	0
53	MG	2A	3215	1/1	0.93	0.38	59,59,59,59	0
53	MG	1A	3323	1/1	0.93	0.16	66,66,66,66	0
53	MG	1A	3054	1/1	0.93	0.65	75,75,75,75	0
53	MG	2A	3080	1/1	0.93	0.27	144,144,144,144	0
53	MG	1A	3330	1/1	0.93	0.36	105,105,105,105	0
53	MG	1a	1861	1/1	0.93	0.07	99,99,99,99	0
53	MG	1A	3547	1/1	0.93	0.19	58,58,58,58	0
53	MG	2A	3318	1/1	0.93	0.09	67,67,67,67	0
53	MG	2A	3067	1/1	0.93	0.15	80,80,80,80	0
53	MG	1A	3693	1/1	0.93	0.19	79,79,79,79	0
53	MG	1A	3714	1/1	0.93	0.44	61,61,61,61	0
53	MG	2A	3378	1/1	0.93	0.12	95,95,95,95	0
53	MG	2a	1702	1/1	0.93	0.18	104,104,104,104	0
53	MG	1a	1760	1/1	0.93	0.16	69,69,69,69	0
53	MG	1a	1823	1/1	0.93	0.31	91,91,91,91	0
53	MG	2A	3408	1/1	0.93	0.24	105,105,105,105	0
53	MG	2D	304	1/1	0.93	0.13	111,111,111,111	0
53	MG	1A	3395	1/1	0.93	0.34	58,58,58,58	0
53	MG	1a	1741	1/1	0.93	0.10	79,79,79,79	0
53	MG	2A	3110	1/1	0.93	0.18	59,59,59,59	0
53	MG	1A	3160	1/1	0.93	0.78	49,49,49,49	0
53	MG	1A	3242	1/1	0.93	0.41	74,74,74,74	0
53	MG	2A	3538	1/1	0.93	0.34	75,75,75,75	0
53	MG	2A	3351	1/1	0.93	0.24	88,88,88,88	0
53	MG	1A	3573	1/1	0.93	0.16	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	2A	3455	1/1	0.93	0.33	88,88,88,88	0
53	MG	1A	3411	1/1	0.93	0.21	68,68,68,68	0
53	MG	1A	3249	1/1	0.93	0.25	58,58,58,58	0
53	MG	2A	3003	1/1	0.93	0.14	90,90,90,90	0
53	MG	2A	3393	1/1	0.93	0.22	65,65,65,65	0
53	MG	1A	3700	1/1	0.93	0.24	54,54,54,54	0
53	MG	1A	3230	1/1	0.93	0.19	28,28,28,28	0
53	MG	2A	3501	1/1	0.93	0.45	60,60,60,60	0
53	MG	2A	3344	1/1	0.93	0.21	93,93,93,93	0
53	MG	2A	3451	1/1	0.93	0.12	64,64,64,64	0
53	MG	1A	3347	1/1	0.93	0.17	69,69,69,69	0
53	MG	2A	3481	1/1	0.93	0.25	99,99,99,99	0
53	MG	1A	3650	1/1	0.93	0.81	62,62,62,62	0
53	MG	1A	3148	1/1	0.93	0.74	47,47,47,47	0
53	MG	1A	3118	1/1	0.93	0.20	91,91,91,91	0
53	MG	2B	204	1/1	0.93	0.64	100,100,100,100	0
53	MG	1A	3283	1/1	0.93	0.21	35,35,35,35	0
53	MG	1N	203	1/1	0.93	0.13	56,56,56,56	0
53	MG	1A	3739	1/1	0.93	0.26	37,37,37,37	0
53	MG	2a	1742	1/1	0.93	0.44	65,65,65,65	0
53	MG	1A	3033	1/1	0.93	0.19	68,68,68,68	0
53	MG	1A	3474	1/1	0.93	0.25	52,52,52,52	0
53	MG	1A	3277	1/1	0.93	0.17	72,72,72,72	0
53	MG	1A	3354	1/1	0.93	0.27	73,73,73,73	0
53	MG	2a	1748	1/1	0.93	0.47	81,81,81,81	0
53	MG	1A	3213	1/1	0.93	0.25	54,54,54,54	0
53	MG	2A	3196	1/1	0.93	0.50	85,85,85,85	0
53	MG	1A	3251	1/1	0.93	0.23	45,45,45,45	0
53	MG	1A	3007	1/1	0.93	0.15	42,42,42,42	0
53	MG	1A	3203	1/1	0.93	0.23	55,55,55,55	0
53	MG	1A	3486	1/1	0.93	0.09	75,75,75,75	0
53	MG	1A	3815	1/1	0.93	0.17	68,68,68,68	0
53	MG	1A	3796	1/1	0.93	0.56	50,50,50,50	0
53	MG	2A	3350	1/1	0.93	0.68	85,85,85,85	0
53	MG	2A	3229	1/1	0.93	0.25	65,65,65,65	0
53	MG	2A	3386	1/1	0.93	0.26	59,59,59,59	0
53	MG	1A	3488	1/1	0.93	0.32	46,46,46,46	0
53	MG	2A	3473	1/1	0.93	0.21	79,79,79,79	0
53	MG	1a	1789	1/1	0.93	0.38	85,85,85,85	0
53	MG	1A	3487	1/1	0.93	0.57	76,76,76,76	0
53	MG	1A	3221	1/1	0.93	0.40	32,32,32,32	0
53	MG	2A	3060	1/1	0.93	0.09	112,112,112,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	1A	3668	1/1	0.93	0.25	74,74,74,74	0
53	MG	1A	3595	1/1	0.93	0.19	47,47,47,47	0
53	MG	1A	3374	1/1	0.93	0.18	33,33,33,33	0
53	MG	1A	3349	1/1	0.93	0.23	33,33,33,33	0
53	MG	2A	3050	1/1	0.93	0.45	101,101,101,101	0
53	MG	1A	3236	1/1	0.93	0.13	61,61,61,61	0
53	MG	1R	202	1/1	0.93	0.41	64,64,64,64	0
53	MG	2A	3418	1/1	0.93	0.23	63,63,63,63	0
53	MG	2A	3332	1/1	0.93	0.14	108,108,108,108	0
53	MG	1a	1756	1/1	0.93	0.53	72,72,72,72	0
53	MG	1A	3324	1/1	0.93	0.18	68,68,68,68	0
53	MG	2A	3513	1/1	0.93	0.27	84,84,84,84	0
53	MG	1A	3499	1/1	0.93	0.20	66,66,66,66	0
53	MG	2a	1765	1/1	0.93	0.25	95,95,95,95	0
53	MG	1A	3414	1/1	0.93	0.19	57,57,57,57	0
53	MG	2A	3047	1/1	0.93	0.22	75,75,75,75	0
53	MG	2A	3562	1/1	0.93	0.14	72,72,72,72	0
53	MG	1a	1882	1/1	0.93	0.32	72,72,72,72	0
53	MG	1A	3028	1/1	0.93	0.14	81,81,81,81	0
53	MG	2B	201	1/1	0.93	0.26	81,81,81,81	0
53	MG	2A	3558	1/1	0.94	0.37	81,81,81,81	0
53	MG	1A	3748	1/1	0.94	0.36	93,93,93,93	0
53	MG	1A	3676	1/1	0.94	0.17	42,42,42,42	0
53	MG	1A	3194	1/1	0.94	0.13	82,82,82,82	0
53	MG	1A	3331	1/1	0.94	0.14	49,49,49,49	0
53	MG	1A	3328	1/1	0.94	0.25	56,56,56,56	0
53	MG	1A	3549	1/1	0.94	0.54	65,65,65,65	0
53	MG	1A	3318	1/1	0.94	0.17	83,83,83,83	0
53	MG	1A	3572	1/1	0.94	0.20	56,56,56,56	0
53	MG	1A	3526	1/1	0.94	0.16	113,113,113,113	0
53	MG	1E	308	1/1	0.94	0.12	67,67,67,67	0
53	MG	1A	3633	1/1	0.94	0.25	80,80,80,80	0
53	MG	2A	3522	1/1	0.94	0.64	110,110,110,110	0
53	MG	1A	3046	1/1	0.94	0.23	90,90,90,90	0
53	MG	13	101	1/1	0.94	0.15	84,84,84,84	0
53	MG	2A	3435	1/1	0.94	0.16	60,60,60,60	0
53	MG	1A	3096	1/1	0.94	0.16	87,87,87,87	0
53	MG	2A	3306	1/1	0.94	0.32	77,77,77,77	0
53	MG	1A	3135	1/1	0.94	0.49	45,45,45,45	0
53	MG	1B	214	1/1	0.94	0.09	82,82,82,82	0
53	MG	2A	3209	1/1	0.94	0.27	71,71,71,71	0
53	MG	2A	3178	1/1	0.94	0.17	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	1A	3140	1/1	0.94	0.30	89,89,89,89	0
53	MG	1A	3598	1/1	0.94	0.12	69,69,69,69	0
53	MG	1A	3433	1/1	0.94	0.35	94,94,94,94	0
53	MG	19	101	1/1	0.94	0.48	40,40,40,40	0
53	MG	1A	3310	1/1	0.94	0.19	86,86,86,86	0
53	MG	1A	3512	1/1	0.94	0.84	58,58,58,58	0
53	MG	1A	3422	1/1	0.94	0.39	62,62,62,62	0
53	MG	1A	3262	1/1	0.94	0.27	36,36,36,36	0
53	MG	2a	1834	1/1	0.94	0.55	46,46,46,46	0
53	MG	1R	201	1/1	0.94	0.16	93,93,93,93	0
53	MG	2T	3003	1/1	0.94	0.19	78,78,78,78	0
53	MG	1D	308	1/1	0.94	0.24	79,79,79,79	0
53	MG	1A	3508	1/1	0.94	0.42	57,57,57,57	0
53	MG	1A	3037	1/1	0.94	0.15	45,45,45,45	0
53	MG	1A	3177	1/1	0.94	0.73	96,96,96,96	0
53	MG	1A	3359	1/1	0.94	0.34	65,65,65,65	0
53	MG	2U	201	1/1	0.94	0.13	79,79,79,79	0
53	MG	1E	301	1/1	0.94	0.17	64,64,64,64	0
53	MG	1A	3122	1/1	0.94	0.22	81,81,81,81	0
53	MG	2A	3048	1/1	0.94	0.14	75,75,75,75	0
53	MG	1E	306	1/1	0.94	0.23	78,78,78,78	0
53	MG	1A	3030	1/1	0.94	0.28	74,74,74,74	0
53	MG	1a	1898	1/1	0.94	0.38	64,64,64,64	0
53	MG	2A	3437	1/1	0.94	0.19	86,86,86,86	0
53	MG	1A	3519	1/1	0.94	0.10	98,98,98,98	0
53	MG	2A	3549	1/1	0.94	0.19	73,73,73,73	0
53	MG	1A	3447	1/1	0.94	0.34	51,51,51,51	0
53	MG	2A	3480	1/1	0.94	0.08	61,61,61,61	0
53	MG	1A	3812	1/1	0.94	0.32	61,61,61,61	0
53	MG	1A	3367	1/1	0.94	0.34	70,70,70,70	0
53	MG	1A	3299	1/1	0.94	0.09	80,80,80,80	0
53	MG	1A	3132	1/1	0.94	0.11	52,52,52,52	0
53	MG	1R	203	1/1	0.94	0.36	67,67,67,67	0
53	MG	10	102	1/1	0.94	0.17	48,48,48,48	0
53	MG	1A	3176	1/1	0.94	0.36	89,89,89,89	0
53	MG	2A	3097	1/1	0.94	0.18	53,53,53,53	0
53	MG	1A	3733	1/1	0.94	0.41	48,48,48,48	0
53	MG	1A	3558	1/1	0.94	0.22	66,66,66,66	0
53	MG	2A	3330	1/1	0.94	0.52	45,45,45,45	0
53	MG	1D	301	1/1	0.94	0.17	61,61,61,61	0
53	MG	1a	1790	1/1	0.94	0.11	65,65,65,65	0
53	MG	1A	3143	1/1	0.94	0.09	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	1A	3455	1/1	0.94	0.13	94,94,94,94	0
53	MG	1a	1800	1/1	0.94	0.09	59,59,59,59	0
53	MG	1A	3107	1/1	0.94	0.67	34,34,34,34	0
53	MG	2A	3411	1/1	0.94	0.25	71,71,71,71	0
53	MG	1A	3590	1/1	0.94	0.11	66,66,66,66	0
53	MG	2A	3146	1/1	0.94	0.39	92,92,92,92	0
53	MG	1A	3806	1/1	0.94	0.19	49,49,49,49	0
53	MG	1A	3677	1/1	0.94	0.13	42,42,42,42	0
53	MG	1a	1802	1/1	0.94	0.24	67,67,67,67	0
53	MG	25	101	1/1	0.94	0.14	99,99,99,99	0
53	MG	1a	1840	1/1	0.94	0.11	99,99,99,99	0
53	MG	2A	3402	1/1	0.94	0.17	76,76,76,76	0
53	MG	1N	201	1/1	0.94	0.28	86,86,86,86	0
53	MG	1A	3239	1/1	0.94	0.26	55,55,55,55	0
53	MG	1a	1893	1/1	0.94	0.15	82,82,82,82	0
53	MG	2A	3058	1/1	0.94	0.24	71,71,71,71	0
53	MG	1a	1869	1/1	0.94	0.48	106,106,106,106	0
53	MG	1A	3091	1/1	0.94	0.20	67,67,67,67	0
53	MG	1A	3468	1/1	0.94	0.31	87,87,87,87	0
53	MG	2A	3090	1/1	0.94	0.10	106,106,106,106	0
53	MG	1A	3292	1/1	0.94	0.25	55,55,55,55	0
53	MG	2A	3482	1/1	0.94	0.40	115,115,115,115	0
53	MG	2a	1705	1/1	0.94	0.08	126,126,126,126	0
53	MG	1E	309	1/1	0.94	0.11	49,49,49,49	0
53	MG	2a	1814	1/1	0.94	0.23	118,118,118,118	0
53	MG	2A	3430	1/1	0.94	0.19	71,71,71,71	0
53	MG	1A	3004	1/1	0.94	0.69	84,84,84,84	0
53	MG	2a	1741	1/1	0.94	0.37	114,114,114,114	0
53	MG	2a	1709	1/1	0.94	0.08	124,124,124,124	0
53	MG	2A	3456	1/1	0.94	0.91	89,89,89,89	0
53	MG	1B	219	1/1	0.94	0.13	67,67,67,67	0
53	MG	2A	3252	1/1	0.94	0.28	61,61,61,61	0
53	MG	1A	3306	1/1	0.94	0.49	73,73,73,73	0
53	MG	2A	3026	1/1	0.94	0.28	119,119,119,119	0
53	MG	1A	3711	1/1	0.94	0.79	69,69,69,69	0
53	MG	1A	3439	1/1	0.94	0.38	61,61,61,61	0
53	MG	1A	3627	1/1	0.94	0.18	89,89,89,89	0
53	MG	2A	3021	1/1	0.94	0.11	66,66,66,66	0
53	MG	1A	3391	1/1	0.94	0.25	77,77,77,77	0
53	MG	2A	3006	1/1	0.94	0.95	73,73,73,73	0
53	MG	2A	3257	1/1	0.94	0.17	77,77,77,77	0
53	MG	1A	3780	1/1	0.94	0.41	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	2A	3470	1/1	0.94	0.26	73,73,73,73	0
53	MG	1A	3707	1/1	0.94	0.20	75,75,75,75	0
53	MG	1A	3448	1/1	0.94	0.43	61,61,61,61	0
53	MG	2A	3181	1/1	0.94	0.25	61,61,61,61	0
53	MG	1A	3250	1/1	0.94	0.38	74,74,74,74	0
53	MG	2A	3189	1/1	0.94	0.15	67,67,67,67	0
53	MG	1A	3280	1/1	0.94	0.28	53,53,53,53	0
53	MG	1A	3686	1/1	0.94	0.20	96,96,96,96	0
53	MG	1A	3472	1/1	0.94	0.16	76,76,76,76	0
53	MG	1A	3215	1/1	0.94	0.24	80,80,80,80	0
53	MG	1A	3424	1/1	0.94	0.39	69,69,69,69	0
53	MG	2A	3534	1/1	0.94	0.28	61,61,61,61	0
53	MG	2A	3492	1/1	0.94	0.07	86,86,86,86	0
53	MG	2A	3192	1/1	0.94	0.42	68,68,68,68	0
53	MG	1H	201	1/1	0.94	0.11	76,76,76,76	0
53	MG	1a	1798	1/1	0.94	0.41	76,76,76,76	0
53	MG	1A	3436	1/1	0.94	0.16	76,76,76,76	0
53	MG	1a	1797	1/1	0.94	0.69	112,112,112,112	0
53	MG	1A	3605	1/1	0.94	0.28	86,86,86,86	0
53	MG	1A	3080	1/1	0.94	0.25	26,26,26,26	0
53	MG	1A	3051	1/1	0.95	0.17	37,37,37,37	0
53	MG	1A	3023	1/1	0.95	0.10	72,72,72,72	0
53	MG	1A	3067	1/1	0.95	0.70	71,71,71,71	0
53	MG	1A	3484	1/1	0.95	0.18	71,71,71,71	0
53	MG	1A	3502	1/1	0.95	0.09	43,43,43,43	0
53	MG	2A	3299	1/1	0.95	0.16	81,81,81,81	0
53	MG	2A	3240	1/1	0.95	0.31	60,60,60,60	0
53	MG	2A	3023	1/1	0.95	0.12	73,73,73,73	0
53	MG	2a	1808	1/1	0.95	0.13	103,103,103,103	0
53	MG	1A	3027	1/1	0.95	0.17	54,54,54,54	0
53	MG	1A	3479	1/1	0.95	0.23	63,63,63,63	0
53	MG	1A	3404	1/1	0.95	0.27	60,60,60,60	0
53	MG	2a	1795	1/1	0.95	0.13	114,114,114,114	0
53	MG	2T	3002	1/1	0.95	0.39	81,81,81,81	0
53	MG	1A	3491	1/1	0.95	0.24	72,72,72,72	0
53	MG	1A	3368	1/1	0.95	0.32	32,32,32,32	0
53	MG	1A	3561	1/1	0.95	0.14	68,68,68,68	0
53	MG	2A	3193	1/1	0.95	0.18	75,75,75,75	0
53	MG	2A	3291	1/1	0.95	0.29	94,94,94,94	0
53	MG	2A	3256	1/1	0.95	0.40	58,58,58,58	0
53	MG	2A	3243	1/1	0.95	0.10	95,95,95,95	0
53	MG	1A	3822	1/1	0.95	0.21	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	1A	3387	1/1	0.95	0.18	64,64,64,64	0
53	MG	1A	3241	1/1	0.95	0.17	73,73,73,73	0
53	MG	1A	3578	1/1	0.95	0.18	49,49,49,49	0
53	MG	1A	3260	1/1	0.95	0.29	50,50,50,50	0
53	MG	1A	3654	1/1	0.95	0.14	55,55,55,55	0
53	MG	1A	3196	1/1	0.95	0.23	34,34,34,34	0
53	MG	1B	207	1/1	0.95	0.33	75,75,75,75	0
57	ZN	26	501	1/1	0.95	0.14	118,118,118,118	0
53	MG	1A	3390	1/1	0.95	0.28	56,56,56,56	0
53	MG	1A	3807	1/1	0.95	0.28	47,47,47,47	0
53	MG	1A	3534	1/1	0.95	0.09	43,43,43,43	0
53	MG	1A	3795	1/1	0.95	0.21	80,80,80,80	0
53	MG	1A	3766	1/1	0.95	0.25	47,47,47,47	0
53	MG	1A	3528	1/1	0.95	0.26	56,56,56,56	0
53	MG	2A	3396	1/1	0.95	0.16	58,58,58,58	0
53	MG	2A	3486	1/1	0.95	0.23	73,73,73,73	0
53	MG	1a	1830	1/1	0.95	0.15	115,115,115,115	0
53	MG	2A	3264	1/1	0.95	0.24	72,72,72,72	0
53	MG	2A	3166	1/1	0.95	0.16	73,73,73,73	0
53	MG	2A	3102	1/1	0.95	0.32	90,90,90,90	0
53	MG	2A	3029	1/1	0.95	0.10	91,91,91,91	0
53	MG	2A	3238	1/1	0.95	0.11	74,74,74,74	0
53	MG	2A	3082	1/1	0.95	0.19	89,89,89,89	0
53	MG	1A	3454	1/1	0.95	0.55	64,64,64,64	0
53	MG	17	101	1/1	0.95	0.19	65,65,65,65	0
53	MG	1A	3010	1/1	0.95	0.35	79,79,79,79	0
53	MG	2A	3385	1/1	0.95	0.33	79,79,79,79	0
53	MG	2a	1843	1/1	0.95	0.31	99,99,99,99	0
53	MG	2A	3051	1/1	0.95	0.14	97,97,97,97	0
53	MG	1A	3073	1/1	0.95	0.35	53,53,53,53	0
53	MG	2A	3527	1/1	0.95	0.79	60,60,60,60	0
53	MG	2A	3271	1/1	0.95	0.30	56,56,56,56	0
53	MG	1A	3343	1/1	0.95	0.41	53,53,53,53	0
53	MG	1A	3048	1/1	0.95	0.23	82,82,82,82	0
53	MG	1A	3119	1/1	0.95	0.33	87,87,87,87	0
53	MG	1A	3434	1/1	0.95	0.19	67,67,67,67	0
53	MG	1A	3184	1/1	0.95	0.27	41,41,41,41	0
53	MG	1A	3339	1/1	0.95	0.12	70,70,70,70	0
53	MG	1A	3162	1/1	0.95	0.13	55,55,55,55	0
53	MG	1A	3551	1/1	0.95	0.30	66,66,66,66	0
53	MG	2A	3387	1/1	0.95	0.14	82,82,82,82	0
53	MG	2A	3176	1/1	0.95	0.25	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	2V	201	1/1	0.95	0.32	63,63,63,63	0
53	MG	1A	3316	1/1	0.95	0.21	87,87,87,87	0
53	MG	1A	3192	1/1	0.95	0.17	59,59,59,59	0
53	MG	2A	3241	1/1	0.95	0.15	83,83,83,83	0
53	MG	1A	3038	1/1	0.95	0.12	50,50,50,50	0
53	MG	1A	3579	1/1	0.95	0.42	55,55,55,55	0
53	MG	1A	3589	1/1	0.95	0.10	63,63,63,63	0
53	MG	2A	3419	1/1	0.95	0.24	54,54,54,54	0
53	MG	1A	3481	1/1	0.95	0.11	67,67,67,67	0
53	MG	1A	3189	1/1	0.95	0.27	50,50,50,50	0
53	MG	1a	1878	1/1	0.95	0.19	82,82,82,82	0
53	MG	2A	3459	1/1	0.95	1.27	92,92,92,92	0
53	MG	1A	3197	1/1	0.95	0.37	70,70,70,70	0
53	MG	1A	3768	1/1	0.95	0.18	96,96,96,96	0
53	MG	2A	3011	1/1	0.95	0.34	63,63,63,63	0
53	MG	10	101	1/1	0.95	0.19	54,54,54,54	0
53	MG	2A	3371	1/1	0.95	0.31	113,113,113,113	0
53	MG	1A	3836	1/1	0.95	0.20	34,34,34,34	0
53	MG	2A	3083	1/1	0.95	0.24	98,98,98,98	0
53	MG	2A	3096	1/1	0.95	0.31	50,50,50,50	0
53	MG	1A	3294	1/1	0.95	0.26	65,65,65,65	0
53	MG	2A	3040	1/1	0.95	0.24	80,80,80,80	0
53	MG	2A	3399	1/1	0.95	0.38	74,74,74,74	0
53	MG	1a	1795	1/1	0.95	0.17	69,69,69,69	0
53	MG	1A	3392	1/1	0.95	0.20	56,56,56,56	0
53	MG	1A	3470	1/1	0.95	0.12	39,39,39,39	0
53	MG	1a	1849	1/1	0.95	0.23	94,94,94,94	0
53	MG	2A	3449	1/1	0.95	0.42	72,72,72,72	0
53	MG	1A	3253	1/1	0.95	0.27	67,67,67,67	0
53	MG	2A	3183	1/1	0.95	0.29	74,74,74,74	0
53	MG	1A	3452	1/1	0.95	0.20	72,72,72,72	0
53	MG	1A	3259	1/1	0.95	0.24	43,43,43,43	0
53	MG	1A	3581	1/1	0.95	0.26	57,57,57,57	0
53	MG	1a	1771	1/1	0.95	0.25	62,62,62,62	0
53	MG	2A	3561	1/1	0.95	0.22	78,78,78,78	0
53	MG	1A	3789	1/1	0.95	0.15	73,73,73,73	0
53	MG	1A	3765	1/1	0.95	0.47	85,85,85,85	0
53	MG	1A	3785	1/1	0.95	0.21	82,82,82,82	0
53	MG	2A	3081	1/1	0.95	0.30	80,80,80,80	0
53	MG	1A	3410	1/1	0.95	0.48	58,58,58,58	0
53	MG	1A	3582	1/1	0.95	0.15	71,71,71,71	0
53	MG	2A	3410	1/1	0.95	0.16	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	1A	3715	1/1	0.95	0.20	52,52,52,52	0
53	MG	1A	3190	1/1	0.95	0.24	85,85,85,85	0
53	MG	1A	3522	1/1	0.95	0.29	58,58,58,58	0
53	MG	2A	3331	1/1	0.95	0.20	103,103,103,103	0
53	MG	1B	218	1/1	0.95	0.22	27,27,27,27	0
53	MG	2A	3434	1/1	0.95	0.22	55,55,55,55	0
53	MG	1A	3503	1/1	0.95	0.23	45,45,45,45	0
53	MG	2A	3260	1/1	0.95	0.15	62,62,62,62	0
53	MG	2A	3440	1/1	0.95	0.33	73,73,73,73	0
53	MG	2A	3425	1/1	0.95	0.76	77,77,77,77	0
53	MG	2a	1830	1/1	0.95	0.22	98,98,98,98	0
53	MG	2A	3427	1/1	0.95	0.43	97,97,97,97	0
53	MG	1A	3705	1/1	0.95	0.34	49,49,49,49	0
53	MG	1A	3261	1/1	0.95	0.21	71,71,71,71	0
53	MG	2A	3529	1/1	0.95	0.45	84,84,84,84	0
53	MG	1a	1863	1/1	0.95	0.24	61,61,61,61	0
53	MG	1W	3001	1/1	0.95	0.20	36,36,36,36	0
53	MG	2A	3524	1/1	0.95	0.13	90,90,90,90	0
53	MG	1A	3409	1/1	0.95	0.23	78,78,78,78	0
53	MG	1A	3513	1/1	0.95	0.27	99,99,99,99	0
53	MG	2A	3433	1/1	0.95	0.25	94,94,94,94	0
53	MG	1A	3791	1/1	0.95	0.19	52,52,52,52	0
53	MG	1X	101	1/1	0.95	0.23	75,75,75,75	0
53	MG	1A	3574	1/1	0.95	0.34	56,56,56,56	0
53	MG	1F	309	1/1	0.95	0.90	92,92,92,92	0
53	MG	1A	3431	1/1	0.95	0.20	68,68,68,68	0
53	MG	1A	3495	1/1	0.95	0.18	63,63,63,63	0
53	MG	1A	3234	1/1	0.95	0.20	68,68,68,68	0
53	MG	1A	3496	1/1	0.95	0.08	69,69,69,69	0
53	MG	2a	1797	1/1	0.95	0.64	79,79,79,79	0
53	MG	2A	3277	1/1	0.95	0.28	82,82,82,82	0
53	MG	2A	3479	1/1	0.95	0.18	119,119,119,119	0
53	MG	1A	3247	1/1	0.95	0.37	55,55,55,55	0
53	MG	2D	301	1/1	0.95	0.23	68,68,68,68	0
53	MG	1A	3735	1/1	0.95	0.21	57,57,57,57	0
53	MG	2A	3547	1/1	0.95	0.24	81,81,81,81	0
53	MG	2F	304	1/1	0.95	0.13	74,74,74,74	0
53	MG	2A	3354	1/1	0.95	0.33	60,60,60,60	0
53	MG	2A	3114	1/1	0.95	0.80	110,110,110,110	0
53	MG	1A	3692	1/1	0.95	0.09	53,53,53,53	0
53	MG	2a	1835	1/1	0.95	0.18	77,77,77,77	0
53	MG	1a	1862	1/1	0.95	0.16	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	2A	3043	1/1	0.95	0.08	114,114,114,114	0
53	MG	1a	1739	1/1	0.95	0.10	80,80,80,80	0
53	MG	1B	202	1/1	0.96	0.16	63,63,63,63	0
53	MG	1A	3273	1/1	0.96	0.30	62,62,62,62	0
53	MG	2A	3112	1/1	0.96	0.17	108,108,108,108	0
53	MG	1A	3181	1/1	0.96	0.13	61,61,61,61	0
53	MG	1A	3640	1/1	0.96	0.24	65,65,65,65	0
53	MG	1a	1864	1/1	0.96	0.37	113,113,113,113	0
53	MG	1A	3245	1/1	0.96	0.26	90,90,90,90	0
53	MG	1B	208	1/1	0.96	0.09	43,43,43,43	0
53	MG	1A	3157	1/1	0.96	0.21	75,75,75,75	0
53	MG	2A	3142	1/1	0.96	0.14	93,93,93,93	0
53	MG	2A	3289	1/1	0.96	0.17	57,57,57,57	0
53	MG	2a	1799	1/1	0.96	1.14	69,69,69,69	0
53	MG	2a	1704	1/1	0.96	0.07	105,105,105,105	0
53	MG	1a	1873	1/1	0.96	0.40	98,98,98,98	0
53	MG	2a	1787	1/1	0.96	0.10	90,90,90,90	0
53	MG	2A	3343	1/1	0.96	0.19	80,80,80,80	0
53	MG	1A	3688	1/1	0.96	0.54	60,60,60,60	0
53	MG	1A	3520	1/1	0.96	0.36	47,47,47,47	0
53	MG	1a	1740	1/1	0.96	0.21	91,91,91,91	0
53	MG	2a	1785	1/1	0.96	0.30	89,89,89,89	0
53	MG	1A	3214	1/1	0.96	0.17	89,89,89,89	0
53	MG	1A	3451	1/1	0.96	0.12	62,62,62,62	0
53	MG	2A	3493	1/1	0.96	0.25	84,84,84,84	0
53	MG	1B	210	1/1	0.96	0.21	49,49,49,49	0
53	MG	1A	3389	1/1	0.96	0.31	76,76,76,76	0
53	MG	1A	3709	1/1	0.96	0.21	30,30,30,30	0
53	MG	2A	3436	1/1	0.96	0.22	91,91,91,91	0
53	MG	1A	3348	1/1	0.96	0.22	72,72,72,72	0
53	MG	2A	3233	1/1	0.96	0.18	56,56,56,56	0
53	MG	1B	216	1/1	0.96	0.16	80,80,80,80	0
53	MG	2R	202	1/1	0.96	0.32	62,62,62,62	0
53	MG	2A	3157	1/1	0.96	0.15	102,102,102,102	0
53	MG	1A	3828	1/1	0.96	0.17	67,67,67,67	0
53	MG	1A	3009	1/1	0.96	0.25	55,55,55,55	0
53	MG	2A	3075	1/1	0.96	0.09	127,127,127,127	0
53	MG	1A	3583	1/1	0.96	0.20	61,61,61,61	0
53	MG	1A	3281	1/1	0.96	0.24	68,68,68,68	0
53	MG	1A	3651	1/1	0.96	0.11	59,59,59,59	0
53	MG	2A	3353	1/1	0.96	0.10	86,86,86,86	0
53	MG	1A	3397	1/1	0.96	0.26	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	1A	3074	1/1	0.96	0.29	80,80,80,80	0
53	MG	2A	3296	1/1	0.96	0.51	82,82,82,82	0
53	MG	1A	3014	1/1	0.96	0.67	81,81,81,81	0
53	MG	2A	3039	1/1	0.96	0.19	59,59,59,59	0
53	MG	1A	3116	1/1	0.96	0.22	85,85,85,85	0
53	MG	1A	3724	1/1	0.96	0.13	44,44,44,44	0
53	MG	1A	3099	1/1	0.96	0.11	37,37,37,37	0
53	MG	1A	3191	1/1	0.96	0.12	62,62,62,62	0
53	MG	2A	3258	1/1	0.96	0.26	71,71,71,71	0
53	MG	1A	3661	1/1	0.96	0.29	109,109,109,109	0
53	MG	2A	3478	1/1	0.96	0.06	81,81,81,81	0
53	MG	1A	3426	1/1	0.96	0.08	69,69,69,69	0
53	MG	2A	3294	1/1	0.96	0.24	103,103,103,103	0
53	MG	2A	3298	1/1	0.96	0.13	87,87,87,87	0
53	MG	1a	1761	1/1	0.96	0.33	103,103,103,103	0
53	MG	1A	3071	1/1	0.96	0.17	83,83,83,83	0
53	MG	1a	1890	1/1	0.96	0.31	67,67,67,67	0
53	MG	2A	3390	1/1	0.96	0.20	87,87,87,87	0
53	MG	1a	1844	1/1	0.96	0.23	86,86,86,86	0
53	MG	2A	3231	1/1	0.96	0.14	53,53,53,53	0
53	MG	2a	1826	1/1	0.96	0.14	89,89,89,89	0
53	MG	1O	8001	1/1	0.96	0.12	75,75,75,75	0
53	MG	1A	3446	1/1	0.96	0.29	64,64,64,64	0
53	MG	1A	3066	1/1	0.96	0.06	93,93,93,93	0
53	MG	1A	3126	1/1	0.96	0.25	57,57,57,57	0
53	MG	1a	1720	1/1	0.96	0.15	127,127,127,127	0
53	MG	2A	3526	1/1	0.96	0.18	78,78,78,78	0
53	MG	1A	3047	1/1	0.96	0.36	52,52,52,52	0
53	MG	1a	1853	1/1	0.96	0.12	86,86,86,86	0
53	MG	1A	3381	1/1	0.96	0.19	44,44,44,44	0
53	MG	1A	3243	1/1	0.96	0.39	49,49,49,49	0
53	MG	2A	3520	1/1	0.96	0.15	81,81,81,81	0
53	MG	2A	3373	1/1	0.96	0.30	95,95,95,95	0
53	MG	1A	3501	1/1	0.96	0.12	67,67,67,67	0
53	MG	1A	3695	1/1	0.96	0.21	36,36,36,36	0
53	MG	2A	3028	1/1	0.96	0.63	51,51,51,51	0
53	MG	1A	3618	1/1	0.96	0.26	60,60,60,60	0
57	ZN	1Y	501	1/1	0.96	0.19	97,97,97,97	0
53	MG	2a	1771	1/1	0.96	0.11	108,108,108,108	0
53	MG	2A	3278	1/1	0.96	0.10	73,73,73,73	0
53	MG	1A	3161	1/1	0.96	0.18	59,59,59,59	0
53	MG	1A	3123	1/1	0.96	0.13	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	1A	3039	1/1	0.96	0.26	60,60,60,60	0
53	MG	2A	3268	1/1	0.96	0.25	44,44,44,44	0
53	MG	1E	304	1/1	0.96	0.19	60,60,60,60	0
53	MG	1A	3416	1/1	0.96	0.14	80,80,80,80	0
53	MG	1A	3612	1/1	0.96	0.44	79,79,79,79	0
53	MG	1A	3254	1/1	0.96	0.18	55,55,55,55	0
53	MG	2F	303	1/1	0.96	0.09	88,88,88,88	0
53	MG	2A	3126	1/1	0.96	0.27	107,107,107,107	0
53	MG	1A	3084	1/1	0.96	0.18	57,57,57,57	0
53	MG	1A	3070	1/1	0.96	0.18	45,45,45,45	0
53	MG	1A	3057	1/1	0.96	0.36	73,73,73,73	0
53	MG	2A	3509	1/1	0.96	0.10	67,67,67,67	0
53	MG	1A	3005	1/1	0.96	0.12	59,59,59,59	0
53	MG	1A	3208	1/1	0.96	0.20	55,55,55,55	0
53	MG	2A	3397	1/1	0.96	0.22	81,81,81,81	0
53	MG	1A	3504	1/1	0.96	0.23	38,38,38,38	0
53	MG	1A	3235	1/1	0.96	0.24	51,51,51,51	0
53	MG	2A	3030	1/1	0.96	0.31	104,104,104,104	0
53	MG	2A	3008	1/1	0.96	0.13	100,100,100,100	0
53	MG	1A	3687	1/1	0.96	0.18	73,73,73,73	0
53	MG	1A	3597	1/1	0.96	0.17	41,41,41,41	0
53	MG	2A	3259	1/1	0.96	0.17	93,93,93,93	0
53	MG	1A	3631	1/1	0.96	0.48	67,67,67,67	0
53	MG	2A	3129	1/1	0.96	0.20	76,76,76,76	0
53	MG	2A	3164	1/1	0.96	0.12	126,126,126,126	0
53	MG	1A	3304	1/1	0.96	0.27	101,101,101,101	0
53	MG	1A	3678	1/1	0.96	0.12	53,53,53,53	0
53	MG	1A	3185	1/1	0.96	0.49	61,61,61,61	0
53	MG	1A	3729	1/1	0.96	0.41	71,71,71,71	0
53	MG	1Q	203	1/1	0.96	0.15	60,60,60,60	0
53	MG	2A	3545	1/1	0.96	0.13	58,58,58,58	0
53	MG	1a	1818	1/1	0.96	0.20	80,80,80,80	0
53	MG	1A	3287	1/1	0.96	0.26	68,68,68,68	0
53	MG	1A	3567	1/1	0.96	0.53	83,83,83,83	0
53	MG	1A	3517	1/1	0.96	0.30	59,59,59,59	0
53	MG	1a	1752	1/1	0.96	0.20	118,118,118,118	0
53	MG	2A	3145	1/1	0.96	0.20	89,89,89,89	0
53	MG	1A	3536	1/1	0.96	0.20	70,70,70,70	0
53	MG	1A	3657	1/1	0.96	0.20	63,63,63,63	0
53	MG	27	101	1/1	0.96	0.46	83,83,83,83	0
53	MG	1A	3267	1/1	0.96	0.17	25,25,25,25	0
53	MG	1a	1728	1/1	0.96	0.18	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	2a	1844	1/1	0.96	1.09	66,66,66,66	0
53	MG	1A	3079	1/1	0.96	0.08	41,41,41,41	0
53	MG	1A	3784	1/1	0.96	0.12	39,39,39,39	0
53	MG	2A	3255	1/1	0.96	0.30	87,87,87,87	0
53	MG	1A	3204	1/1	0.96	0.14	99,99,99,99	0
53	MG	1a	1842	1/1	0.96	0.15	76,76,76,76	0
53	MG	1A	3229	1/1	0.96	0.35	66,66,66,66	0
53	MG	1A	3771	1/1	0.96	0.15	25,25,25,25	0
53	MG	1A	3372	1/1	0.96	0.22	83,83,83,83	0
53	MG	2A	3491	1/1	0.96	0.13	66,66,66,66	0
53	MG	2A	3154	1/1	0.96	0.40	108,108,108,108	0
53	MG	1A	3034	1/1	0.96	0.20	34,34,34,34	0
53	MG	1A	3012	1/1	0.96	0.20	69,69,69,69	0
53	MG	2A	3362	1/1	0.96	0.39	82,82,82,82	0
53	MG	1A	3145	1/1	0.96	0.21	66,66,66,66	0
53	MG	1A	3400	1/1	0.96	0.44	68,68,68,68	0
53	MG	1A	3839	1/1	0.96	0.68	72,72,72,72	0
53	MG	2A	3521	1/1	0.96	0.15	79,79,79,79	0
53	MG	1A	3383	1/1	0.96	0.28	43,43,43,43	0
53	MG	1a	1793	1/1	0.96	0.52	81,81,81,81	0
53	MG	2A	3305	1/1	0.96	0.16	84,84,84,84	0
53	MG	1A	3357	1/1	0.96	0.24	37,37,37,37	0
53	MG	1a	1876	1/1	0.96	0.14	105,105,105,105	0
53	MG	1A	3681	1/1	0.96	0.19	87,87,87,87	0
53	MG	2A	3372	1/1	0.96	0.18	42,42,42,42	0
53	MG	2A	3431	1/1	0.96	0.19	101,101,101,101	0
53	MG	1A	3312	1/1	0.96	0.27	55,55,55,55	0
53	MG	2A	3420	1/1	0.96	0.15	65,65,65,65	0
53	MG	1A	3813	1/1	0.96	0.31	37,37,37,37	0
53	MG	1A	3428	1/1	0.96	0.22	85,85,85,85	0
53	MG	1A	3621	1/1	0.96	0.18	74,74,74,74	0
53	MG	1A	3407	1/1	0.96	0.14	78,78,78,78	0
53	MG	1B	209	1/1	0.96	0.21	33,33,33,33	0
53	MG	2A	3199	1/1	0.96	0.37	65,65,65,65	0
53	MG	1A	3553	1/1	0.96	0.61	86,86,86,86	0
53	MG	2A	3383	1/1	0.96	0.30	78,78,78,78	0
53	MG	1A	3500	1/1	0.96	0.17	65,65,65,65	0
53	MG	1A	3219	1/1	0.96	0.23	62,62,62,62	0
53	MG	2A	3345	1/1	0.96	0.13	52,52,52,52	0
53	MG	1A	3112	1/1	0.97	0.20	44,44,44,44	0
53	MG	1A	3659	1/1	0.97	0.20	56,56,56,56	0
53	MG	1a	1833	1/1	0.97	0.13	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	1A	3505	1/1	0.97	0.21	78,78,78,78	0
53	MG	1A	3365	1/1	0.97	0.29	42,42,42,42	0
53	MG	1A	3226	1/1	0.97	0.33	68,68,68,68	0
53	MG	2A	3089	1/1	0.97	0.11	101,101,101,101	0
53	MG	2A	3222	1/1	0.97	0.34	65,65,65,65	0
53	MG	1A	3198	1/1	0.97	0.28	38,38,38,38	0
53	MG	1a	1757	1/1	0.97	0.19	123,123,123,123	0
53	MG	1A	3199	1/1	0.97	0.23	39,39,39,39	0
53	MG	1A	3255	1/1	0.97	0.19	34,34,34,34	0
53	MG	1A	3823	1/1	0.97	0.36	70,70,70,70	0
53	MG	1P	201	1/1	0.97	0.32	60,60,60,60	0
53	MG	2a	1723	1/1	0.97	0.37	120,120,120,120	0
53	MG	2O	201	1/1	0.97	0.21	66,66,66,66	0
53	MG	1A	3334	1/1	0.97	0.36	59,59,59,59	0
53	MG	1A	3120	1/1	0.97	0.25	74,74,74,74	0
53	MG	2A	3454	1/1	0.97	0.17	69,69,69,69	0
53	MG	1a	1783	1/1	0.97	0.82	63,63,63,63	0
53	MG	2A	3216	1/1	0.97	0.21	79,79,79,79	0
53	MG	2A	3274	1/1	0.97	0.24	81,81,81,81	0
53	MG	1A	3559	1/1	0.97	0.26	47,47,47,47	0
53	MG	2A	3487	1/1	0.97	0.17	60,60,60,60	0
53	MG	2A	3466	1/1	0.97	0.18	61,61,61,61	0
53	MG	1a	1888	1/1	0.97	0.37	68,68,68,68	0
53	MG	1A	3020	1/1	0.97	0.38	58,58,58,58	0
53	MG	1A	3586	1/1	0.97	0.21	57,57,57,57	0
53	MG	2A	3175	1/1	0.97	0.18	70,70,70,70	0
53	MG	1A	3311	1/1	0.97	0.15	65,65,65,65	0
53	MG	17	103	1/1	0.97	0.19	66,66,66,66	0
53	MG	1A	3622	1/1	0.97	0.05	44,44,44,44	0
53	MG	1f	8001	1/1	0.97	0.21	78,78,78,78	0
53	MG	1a	1722	1/1	0.97	0.10	114,114,114,114	0
53	MG	1A	3167	1/1	0.97	0.20	80,80,80,80	0
53	MG	1P	202	1/1	0.97	0.14	65,65,65,65	0
53	MG	2A	3447	1/1	0.97	0.45	81,81,81,81	0
53	MG	1A	3497	1/1	0.97	0.13	101,101,101,101	0
53	MG	1A	3591	1/1	0.97	0.29	56,56,56,56	0
53	MG	1A	3295	1/1	0.97	0.23	64,64,64,64	0
53	MG	1A	3344	1/1	0.97	0.38	48,48,48,48	0
53	MG	1A	3450	1/1	0.97	0.30	41,41,41,41	0
53	MG	1A	3467	1/1	0.97	0.19	30,30,30,30	0
53	MG	1A	3596	1/1	0.97	0.25	45,45,45,45	0
53	MG	2A	3169	1/1	0.97	0.43	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	2a	1820	1/1	0.97	0.22	126,126,126,126	0
53	MG	1A	3673	1/1	0.97	0.06	48,48,48,48	0
53	MG	2A	3143	1/1	0.97	0.13	107,107,107,107	0
53	MG	2A	3187	1/1	0.97	0.20	69,69,69,69	0
53	MG	1A	3808	1/1	0.97	0.30	59,59,59,59	0
53	MG	1A	3183	1/1	0.97	0.10	85,85,85,85	0
53	MG	2A	3287	1/1	0.97	0.26	65,65,65,65	0
53	MG	1A	3697	1/1	0.97	0.42	75,75,75,75	0
53	MG	2A	3563	1/1	0.97	0.33	63,63,63,63	0
53	MG	1A	3361	1/1	0.97	0.22	59,59,59,59	0
53	MG	1A	3335	1/1	0.97	0.23	45,45,45,45	0
53	MG	1A	3529	1/1	0.97	0.44	50,50,50,50	0
53	MG	1A	3127	1/1	0.97	0.17	69,69,69,69	0
53	MG	1A	3625	1/1	0.97	0.17	67,67,67,67	0
53	MG	2A	3438	1/1	0.97	0.22	100,100,100,100	0
53	MG	2A	3057	1/1	0.97	0.66	87,87,87,87	0
53	MG	2a	1813	1/1	0.97	0.31	97,97,97,97	0
53	MG	1D	313	1/1	0.97	0.07	67,67,67,67	0
53	MG	1V	203	1/1	0.97	0.15	46,46,46,46	0
53	MG	1A	3475	1/1	0.97	0.24	36,36,36,36	0
53	MG	1A	3305	1/1	0.97	0.30	31,31,31,31	0
53	MG	1a	1772	1/1	0.97	0.27	88,88,88,88	0
53	MG	1A	3794	1/1	0.97	0.21	66,66,66,66	0
53	MG	2A	3370	1/1	0.97	0.14	63,63,63,63	0
53	MG	2A	3452	1/1	0.97	0.28	79,79,79,79	0
57	ZN	15	101	1/1	0.97	0.21	74,74,74,74	0
53	MG	2A	3159	1/1	0.97	0.20	84,84,84,84	0
53	MG	1A	3291	1/1	0.97	0.22	37,37,37,37	0
53	MG	1A	3619	1/1	0.97	0.36	82,82,82,82	0
53	MG	1A	3814	1/1	0.97	0.18	44,44,44,44	0
53	MG	1A	3465	1/1	0.97	0.14	89,89,89,89	0
53	MG	2A	3162	1/1	0.97	0.32	78,78,78,78	0
53	MG	1A	3742	1/1	0.97	0.13	53,53,53,53	0
53	MG	1A	3437	1/1	0.97	0.28	58,58,58,58	0
53	MG	2A	3391	1/1	0.97	0.38	67,67,67,67	0
53	MG	1A	3720	1/1	0.97	0.15	61,61,61,61	0
53	MG	2B	202	1/1	0.97	0.14	134,134,134,134	0
53	MG	1A	3819	1/1	0.97	0.24	42,42,42,42	0
53	MG	1A	3585	1/1	0.97	0.16	82,82,82,82	0
53	MG	1a	1780	1/1	0.97	0.18	77,77,77,77	0
53	MG	1A	3224	1/1	0.97	0.48	77,77,77,77	0
53	MG	2A	3078	1/1	0.97	0.40	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	1A	3838	1/1	0.97	0.37	66,66,66,66	0
53	MG	2A	3220	1/1	0.97	0.31	76,76,76,76	0
53	MG	1D	305	1/1	0.97	0.25	45,45,45,45	0
53	MG	1A	3286	1/1	0.97	0.17	67,67,67,67	0
53	MG	1A	3256	1/1	0.97	0.15	63,63,63,63	0
53	MG	2a	1750	1/1	0.97	0.17	119,119,119,119	0
53	MG	1A	3269	1/1	0.97	0.14	71,71,71,71	0
53	MG	2A	3333	1/1	0.97	0.30	72,72,72,72	0
53	MG	1A	3268	1/1	0.97	0.08	41,41,41,41	0
53	MG	1A	3644	1/1	0.97	0.17	66,66,66,66	0
53	MG	1A	3603	1/1	0.97	0.17	69,69,69,69	0
53	MG	1A	3231	1/1	0.97	0.42	76,76,76,76	0
53	MG	1A	3200	1/1	0.97	0.32	57,57,57,57	0
53	MG	2A	3034	1/1	0.97	0.10	96,96,96,96	0
53	MG	1D	309	1/1	0.97	0.18	77,77,77,77	0
53	MG	2A	3301	1/1	0.97	0.16	66,66,66,66	0
53	MG	1A	3647	1/1	0.97	0.22	65,65,65,65	0
53	MG	1A	3081	1/1	0.97	0.20	70,70,70,70	0
53	MG	2W	201	1/1	0.97	0.17	64,64,64,64	0
53	MG	1A	3649	1/1	0.97	0.23	49,49,49,49	0
53	MG	1a	1774	1/1	0.97	0.08	111,111,111,111	0
53	MG	1A	3672	1/1	0.97	0.43	35,35,35,35	0
53	MG	1A	3743	1/1	0.97	0.27	103,103,103,103	0
53	MG	1A	3353	1/1	0.97	0.23	63,63,63,63	0
53	MG	1A	3340	1/1	0.97	0.22	38,38,38,38	0
53	MG	1A	3554	1/1	0.97	0.20	43,43,43,43	0
57	ZN	16	501	1/1	0.97	0.18	68,68,68,68	0
53	MG	1A	3703	1/1	0.97	0.36	61,61,61,61	0
53	MG	1A	3716	1/1	0.97	0.24	83,83,83,83	0
53	MG	1A	3272	1/1	0.97	0.23	46,46,46,46	0
53	MG	1A	3656	1/1	0.97	0.51	83,83,83,83	0
53	MG	1A	3831	1/1	0.97	0.26	41,41,41,41	0
53	MG	1A	3445	1/1	0.97	0.16	71,71,71,71	0
53	MG	1a	1706	1/1	0.97	0.10	105,105,105,105	0
53	MG	2A	3202	1/1	0.97	0.17	54,54,54,54	0
53	MG	1A	3719	1/1	0.97	0.11	73,73,73,73	0
53	MG	28	8001	1/1	0.97	0.29	119,119,119,119	0
53	MG	1A	3373	1/1	0.98	0.13	54,54,54,54	0
53	MG	1a	1773	1/1	0.98	0.58	51,51,51,51	0
53	MG	1A	3803	1/1	0.98	0.10	50,50,50,50	0
53	MG	1A	3100	1/1	0.98	0.20	101,101,101,101	0
53	MG	1A	3378	1/1	0.98	0.14	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	SF4	1d	501	8/8	0.98	0.15	116,146,171,175	0
53	MG	2A	3014	1/1	0.98	0.16	88,88,88,88	0
53	MG	2a	1724	1/1	0.98	0.25	103,103,103,103	0
53	MG	2A	3442	1/1	0.98	0.28	89,89,89,89	0
53	MG	1B	203	1/1	0.98	0.13	59,59,59,59	0
53	MG	1A	3314	1/1	0.98	0.12	62,62,62,62	0
53	MG	2A	3312	1/1	0.98	0.11	104,104,104,104	0
53	MG	2A	3072	1/1	0.98	0.24	72,72,72,72	0
53	MG	1A	3228	1/1	0.98	0.29	28,28,28,28	0
57	ZN	25	102	1/1	0.98	0.20	103,103,103,103	0
53	MG	1a	1723	1/1	0.98	0.29	79,79,79,79	0
53	MG	1a	1721	1/1	0.98	0.11	114,114,114,114	0
53	MG	2A	3548	1/1	0.98	0.15	77,77,77,77	0
53	MG	2A	3101	1/1	0.98	0.23	93,93,93,93	0
53	MG	1a	1769	1/1	0.98	0.24	129,129,129,129	0
53	MG	1A	3246	1/1	0.98	0.21	46,46,46,46	0
53	MG	1A	3150	1/1	0.98	0.17	66,66,66,66	0
53	MG	2a	1827	1/1	0.98	0.32	68,68,68,68	0
53	MG	1A	3068	1/1	0.98	0.13	83,83,83,83	0
53	MG	2A	3554	1/1	0.98	0.16	68,68,68,68	0
53	MG	2A	3049	1/1	0.98	0.15	78,78,78,78	0
53	MG	1A	3168	1/1	0.98	0.14	88,88,88,88	0
53	MG	1A	3017	1/1	0.98	0.14	85,85,85,85	0
53	MG	2A	3303	1/1	0.98	0.09	64,64,64,64	0
53	MG	1A	3178	1/1	0.98	0.20	71,71,71,71	0
53	MG	2A	3349	1/1	0.98	0.39	77,77,77,77	0
53	MG	2A	3327	1/1	0.98	0.22	82,82,82,82	0
53	MG	1A	3824	1/1	0.98	0.48	65,65,65,65	0
53	MG	2A	3489	1/1	0.98	0.12	74,74,74,74	0
53	MG	1A	3527	1/1	0.98	0.20	56,56,56,56	0
53	MG	2A	3514	1/1	0.98	0.34	66,66,66,66	0
53	MG	1A	3539	1/1	0.98	0.18	53,53,53,53	0
53	MG	1N	202	1/1	0.98	0.16	67,67,67,67	0
53	MG	1a	1737	1/1	0.98	0.16	114,114,114,114	0
53	MG	1A	3817	1/1	0.98	0.30	34,34,34,34	0
53	MG	2A	3059	1/1	0.98	0.15	84,84,84,84	0
53	MG	2A	3016	1/1	0.98	0.14	105,105,105,105	0
53	MG	1A	3552	1/1	0.98	0.18	36,36,36,36	0
53	MG	1A	3740	1/1	0.98	0.38	33,33,33,33	0
53	MG	1A	3337	1/1	0.98	0.25	53,53,53,53	0
53	MG	1a	1894	1/1	0.98	0.16	53,53,53,53	0
53	MG	1A	3078	1/1	0.98	0.26	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	1A	3355	1/1	0.98	0.10	47,47,47,47	0
53	MG	1A	3220	1/1	0.98	0.24	46,46,46,46	0
53	MG	1A	3016	1/1	0.98	0.46	73,73,73,73	0
53	MG	1D	311	1/1	0.98	0.15	71,71,71,71	0
53	MG	2R	201	1/1	0.98	0.11	93,93,93,93	0
53	MG	1A	3546	1/1	0.98	0.35	43,43,43,43	0
53	MG	1A	3217	1/1	0.98	0.17	69,69,69,69	0
53	MG	2A	3281	1/1	0.98	0.22	57,57,57,57	0
53	MG	1A	3043	1/1	0.98	0.09	70,70,70,70	0
53	MG	1A	3202	1/1	0.98	0.17	49,49,49,49	0
53	MG	1D	302	1/1	0.98	0.41	58,58,58,58	0
53	MG	1A	3103	1/1	0.98	0.19	88,88,88,88	0
53	MG	2A	3012	1/1	0.98	0.13	101,101,101,101	0
53	MG	2A	3015	1/1	0.98	0.16	69,69,69,69	0
53	MG	1A	3158	1/1	0.98	0.22	70,70,70,70	0
53	MG	1A	3704	1/1	0.98	0.26	47,47,47,47	0
53	MG	2A	3239	1/1	0.98	0.18	74,74,74,74	0
53	MG	1A	3827	1/1	0.98	0.29	72,72,72,72	0
53	MG	1A	3617	1/1	0.98	0.10	77,77,77,77	0
58	SF4	2d	501	8/8	0.98	0.10	118,150,171,175	0
53	MG	1A	3121	1/1	0.98	0.15	65,65,65,65	0
53	MG	1A	3174	1/1	0.98	0.21	78,78,78,78	0
53	MG	1A	3297	1/1	0.98	0.20	65,65,65,65	0
53	MG	1Z	8001	1/1	0.98	0.07	54,54,54,54	0
53	MG	1a	1808	1/1	0.98	0.12	87,87,87,87	0
53	MG	2a	1788	1/1	0.98	0.17	96,96,96,96	0
53	MG	1A	3115	1/1	0.98	0.16	45,45,45,45	0
53	MG	1A	3599	1/1	0.98	0.28	57,57,57,57	0
53	MG	1A	3744	1/1	0.98	0.48	73,73,73,73	0
53	MG	2A	3104	1/1	0.98	0.21	192,192,192,192	0
53	MG	1A	3802	1/1	0.98	0.37	54,54,54,54	0
53	MG	1A	3173	1/1	0.98	0.22	79,79,79,79	0
53	MG	1A	3342	1/1	0.98	0.23	62,62,62,62	0
53	MG	1A	3804	1/1	0.98	0.16	67,67,67,67	0
53	MG	2A	3251	1/1	0.98	0.24	41,41,41,41	0
53	MG	1E	305	1/1	0.98	0.32	32,32,32,32	0
53	MG	2A	3147	1/1	0.98	0.32	86,86,86,86	0
53	MG	1A	3835	1/1	0.98	0.28	56,56,56,56	0
53	MG	2a	1780	1/1	0.98	0.11	74,74,74,74	0
53	MG	1D	310	1/1	0.98	0.12	92,92,92,92	0
53	MG	1A	3151	1/1	0.98	0.25	58,58,58,58	0
53	MG	1A	3111	1/1	0.98	0.20	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	1A	3125	1/1	0.98	0.24	65,65,65,65	0
53	MG	1a	1750	1/1	0.98	0.20	118,118,118,118	0
53	MG	1A	3077	1/1	0.98	0.25	83,83,83,83	0
53	MG	1A	3456	1/1	0.98	0.10	52,52,52,52	0
53	MG	1A	3147	1/1	0.98	0.21	65,65,65,65	0
53	MG	1A	3138	1/1	0.98	0.18	68,68,68,68	0
53	MG	1A	3063	1/1	0.98	0.26	84,84,84,84	0
53	MG	1A	3244	1/1	0.98	0.19	68,68,68,68	0
53	MG	1F	304	1/1	0.98	0.35	49,49,49,49	0
53	MG	1a	1749	1/1	0.98	0.39	95,95,95,95	0
53	MG	1A	3556	1/1	0.99	0.22	49,49,49,49	0
53	MG	1A	3094	1/1	0.99	0.16	51,51,51,51	0
53	MG	2A	3009	1/1	0.99	0.14	71,71,71,71	0
53	MG	1A	3694	1/1	0.99	0.14	72,72,72,72	0
53	MG	2A	3045	1/1	0.99	0.20	92,92,92,92	0
53	MG	2A	3156	1/1	0.99	0.33	74,74,74,74	0
53	MG	2A	3182	1/1	0.99	0.17	86,86,86,86	0
53	MG	2F	302	1/1	0.99	0.20	75,75,75,75	0
53	MG	1A	3533	1/1	0.99	0.27	64,64,64,64	0
53	MG	2A	3211	1/1	0.99	0.18	62,62,62,62	0
53	MG	1A	3061	1/1	0.99	0.24	56,56,56,56	0
53	MG	1A	3060	1/1	0.99	0.17	45,45,45,45	0
53	MG	1A	3809	1/1	0.99	0.21	47,47,47,47	0
53	MG	1A	3833	1/1	0.99	0.14	59,59,59,59	0
53	MG	2A	3508	1/1	0.99	0.04	86,86,86,86	0
53	MG	2A	3556	1/1	0.99	0.14	62,62,62,62	0
53	MG	2A	3135	1/1	0.99	0.29	109,109,109,109	0
53	MG	2A	3107	1/1	0.99	0.20	99,99,99,99	0
53	MG	1A	3170	1/1	0.99	0.25	59,59,59,59	0
53	MG	1A	3587	1/1	0.99	0.32	50,50,50,50	0
57	ZN	19	102	1/1	0.99	0.28	67,67,67,67	0
53	MG	2A	3210	1/1	0.99	0.22	62,62,62,62	0
53	MG	2A	3001	1/1	0.99	0.11	98,98,98,98	0
53	MG	2E	301	1/1	0.99	0.19	52,52,52,52	0
53	MG	2A	3052	1/1	0.99	0.20	65,65,65,65	0
53	MG	1A	3186	1/1	0.99	0.16	70,70,70,70	0
53	MG	1A	3645	1/1	0.99	0.13	61,61,61,61	0
53	MG	1A	3108	1/1	0.99	0.10	60,60,60,60	0
53	MG	1A	3076	1/1	0.99	0.10	78,78,78,78	0
53	MG	2A	3542	1/1	0.99	0.21	71,71,71,71	0
53	MG	1A	3514	1/1	0.99	0.12	70,70,70,70	0
53	MG	1A	3036	1/1	0.99	0.14	57,57,57,57	0

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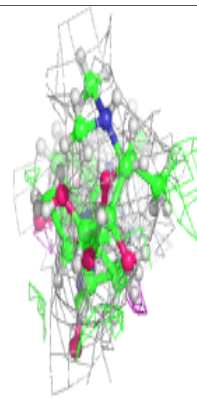
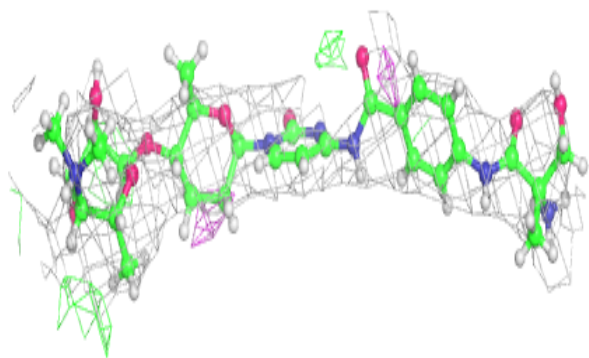
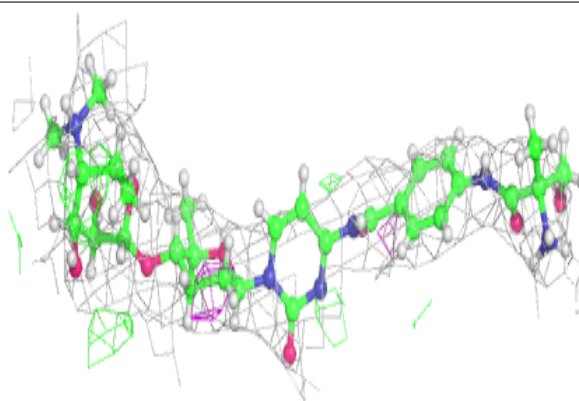
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	1A	3274	1/1	0.99	0.24	56,56,56,56	0
53	MG	1A	3345	1/1	0.99	0.23	47,47,47,47	0
53	MG	1A	3149	1/1	1.00	0.20	55,55,55,55	0
53	MG	1A	3056	1/1	1.00	0.27	78,78,78,78	0
53	MG	1A	3035	1/1	1.00	0.14	57,57,57,57	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 FSD 2A 3553:**

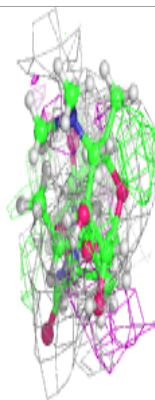
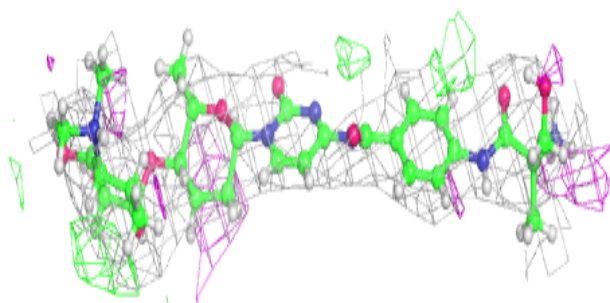
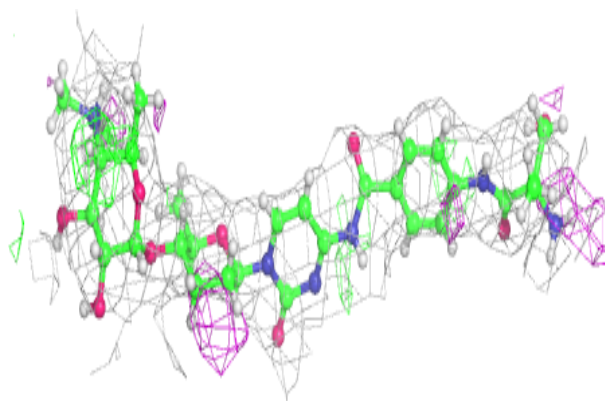
2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around FSD 1A 3801:**

$2mF_o - DF_c$  (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.