



Full wwPDB X-ray Structure Validation 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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

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

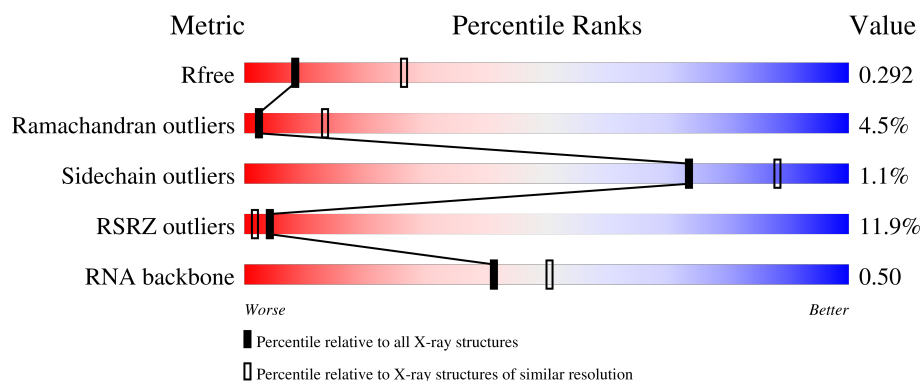
1 Overall quality at a glance

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 ≥ 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>

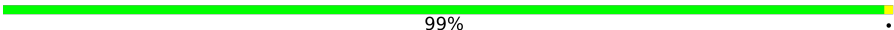

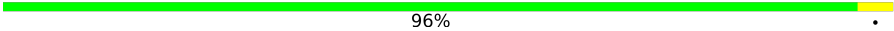

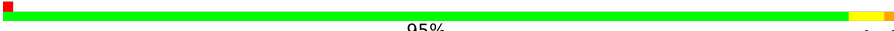

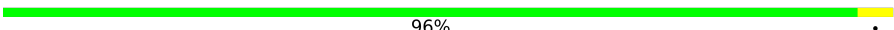

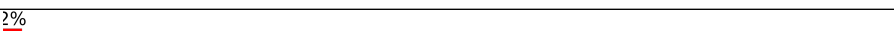
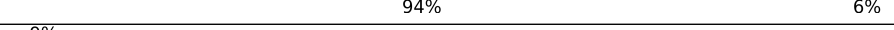
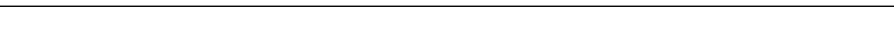
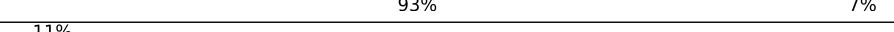


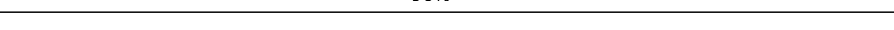
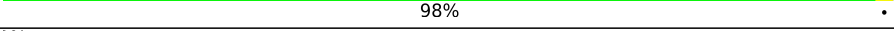
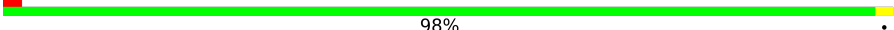

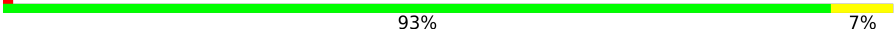


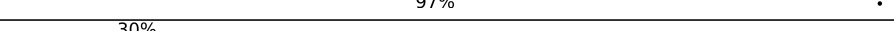


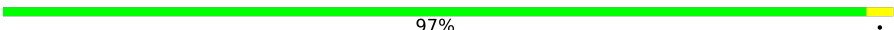
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Mol	Chain	Length	Quality of chain
3	2D	275	% 97% .
4	1E	204	% 99% .
4	2E	204	5% 97% .
5	1F	203	% 96% .
5	2F	203	3% 96% .
6	1G	181	16% 96% .
6	2G	181	30% 93% 7% .
7	1H	174	% 97% .
7	2H	174	18% 93% 6% .
8	1I	147	11% 92% 8% .
8	2I	147	14% 92% 7% .
9	1N	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	<div> <div>6%</div> <div>100%</div> </div>
29	17	48	<div> <div>2%</div> <div>96%</div> <div>.</div> </div>
29	27	48	<div> <div>98%</div> <div>.</div> </div>
30	18	64	<div> <div>98%</div> <div>.</div> </div>
30	28	64	<div> <div>100%</div> </div>
31	19	37	<div> <div>100%</div> </div>
31	29	37	<div> <div>8%</div> <div>97%</div> <div>.</div> </div>
32	1a	2331	<div> <div>14%</div> <div>52%</div> <div>12%</div> <div>36%</div> </div>
32	2a	2331	<div> <div>15%</div> <div>52%</div> <div>12%</div> <div>35%</div> </div>
33	1b	231	<div> <div>13%</div> <div>86%</div> <div>13%</div> <div>.</div> </div>
33	2b	231	<div> <div>18%</div> <div>91%</div> <div>9%</div> </div>
34	1c	206	<div> <div>33%</div> <div>95%</div> <div>5%</div> </div>
34	2c	206	<div> <div>33%</div> <div>94%</div> <div>6%</div> </div>
35	1d	208	<div> <div>12%</div> <div>93%</div> <div>7%</div> </div>
35	2d	208	<div> <div>10%</div> <div>96%</div> <div>.</div> </div>
36	1e	148	<div> <div>7%</div> <div>95%</div> <div>5%</div> </div>
36	2e	148	<div> <div>9%</div> <div>95%</div> <div>5%</div> </div>
37	1f	100	<div> <div>5%</div> <div>97%</div> <div>.</div> </div>
37	2f	100	<div> <div>9%</div> <div>96%</div> <div>..</div> </div>
38	1g	155	<div> <div>40%</div> <div>96%</div> <div>.</div> </div>
38	2g	155	<div> <div>41%</div> <div>93%</div> <div>7%</div> </div>
39	1h	137	<div> <div>%</div> <div>93%</div> <div>7%</div> </div>
39	2h	137	<div> <div>4%</div> <div>92%</div> <div>8%</div> </div>
40	1i	127	<div> <div>51%</div> <div>94%</div> <div>6%</div> </div>
40	2i	127	<div> <div>39%</div> <div>93%</div> <div>6%</div> <div>..</div> </div>

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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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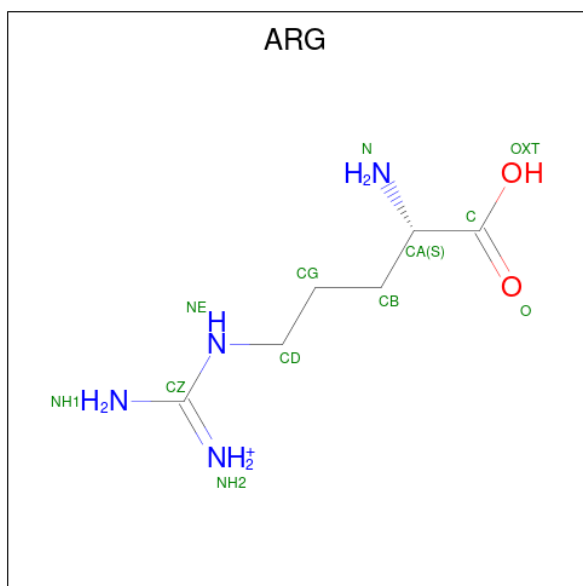
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
53	1G	3	Total 3	Mg 3	0	0
53	2O	2	Total 2	Mg 2	0	0
53	11	3	Total 3	Mg 3	0	0
53	1d	2	Total 2	Mg 2	0	0
53	2n	1	Total 1	Mg 1	0	0
53	1H	3	Total 3	Mg 3	0	0
53	21	1	Total 1	Mg 1	0	0
53	2Y	1	Total 1	Mg 1	0	0
53	2R	2	Total 2	Mg 2	0	0
53	1Z	2	Total 2	Mg 2	0	0
53	2D	7	Total 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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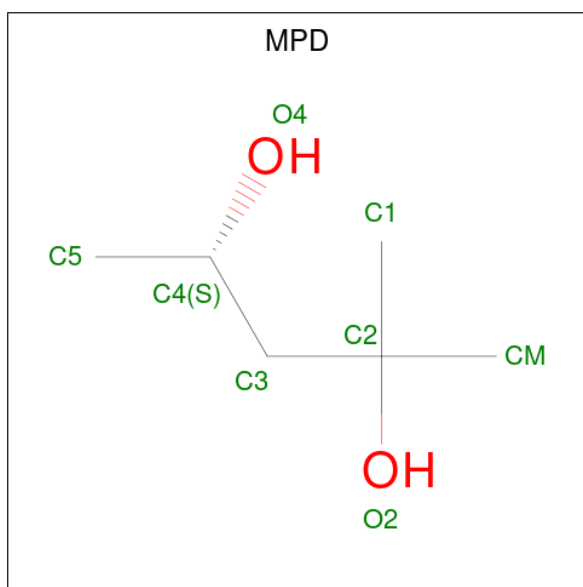
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
53	1Q	3	Total	Mg	0	0
			3	3		
53	2A	561	Total	Mg	0	0
			561	561		
53	1h	1	Total	Mg	0	0
			1	1		
53	2Z	1	Total	Mg	0	0
			1	1		
53	1B	24	Total	Mg	0	0
			24	24		

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



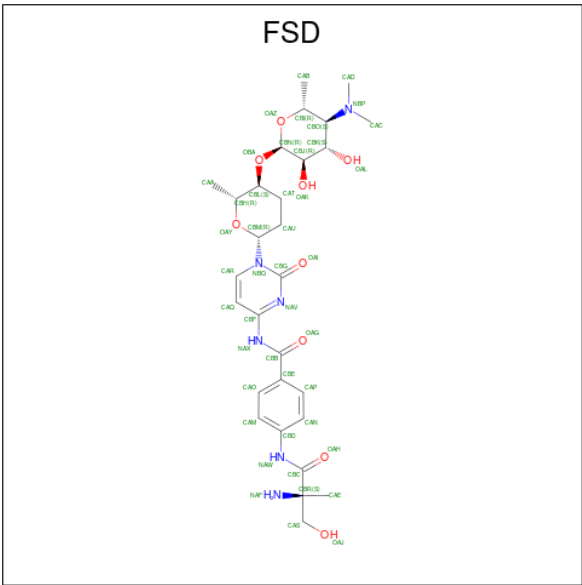
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
54	1A	1	Total	C	N	O	0	0
			12	6	4	2		
54	1B	1	Total	C	N	O	0	0
			12	6	4	2		

- 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: Fe₄S₄).



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

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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

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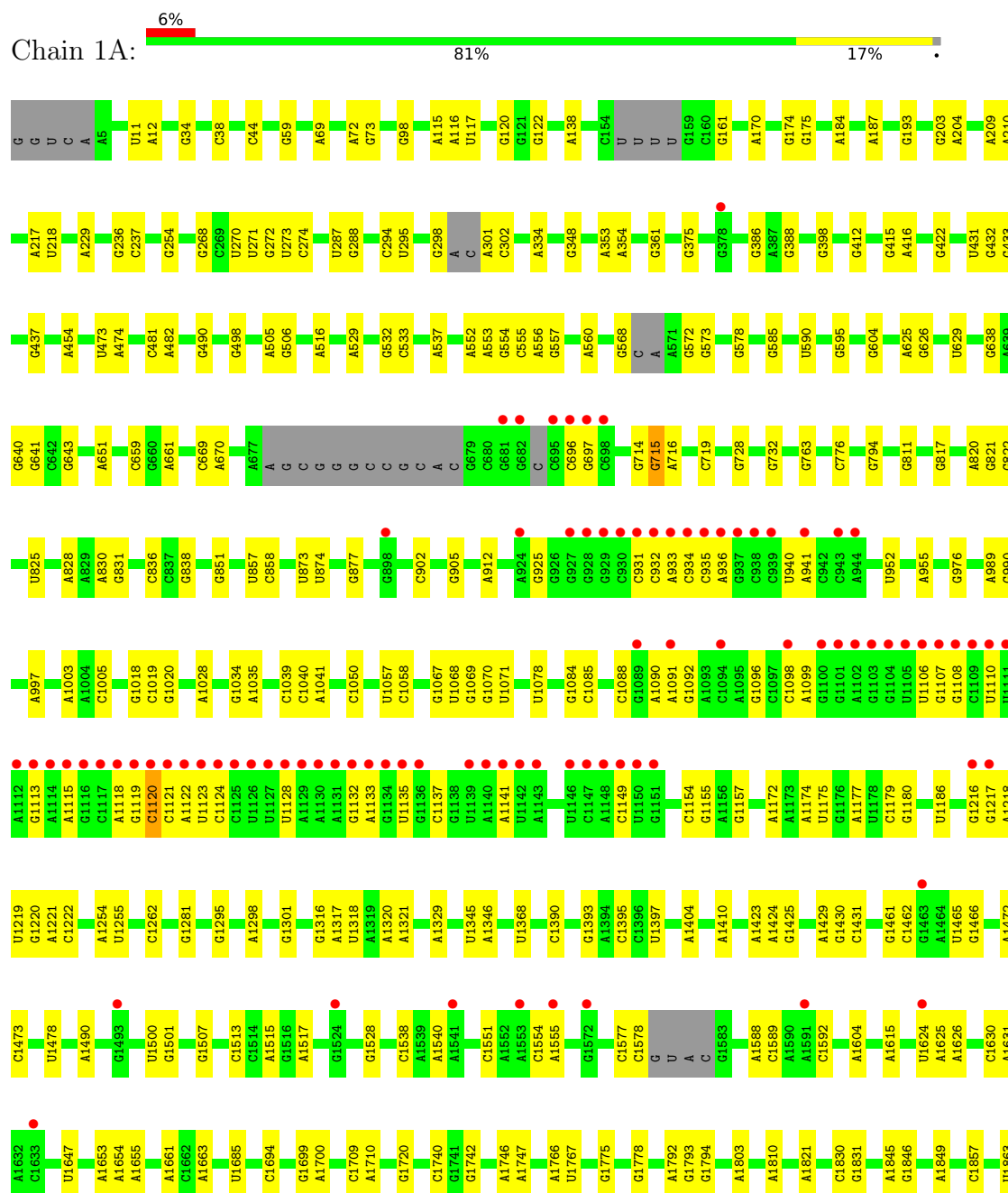
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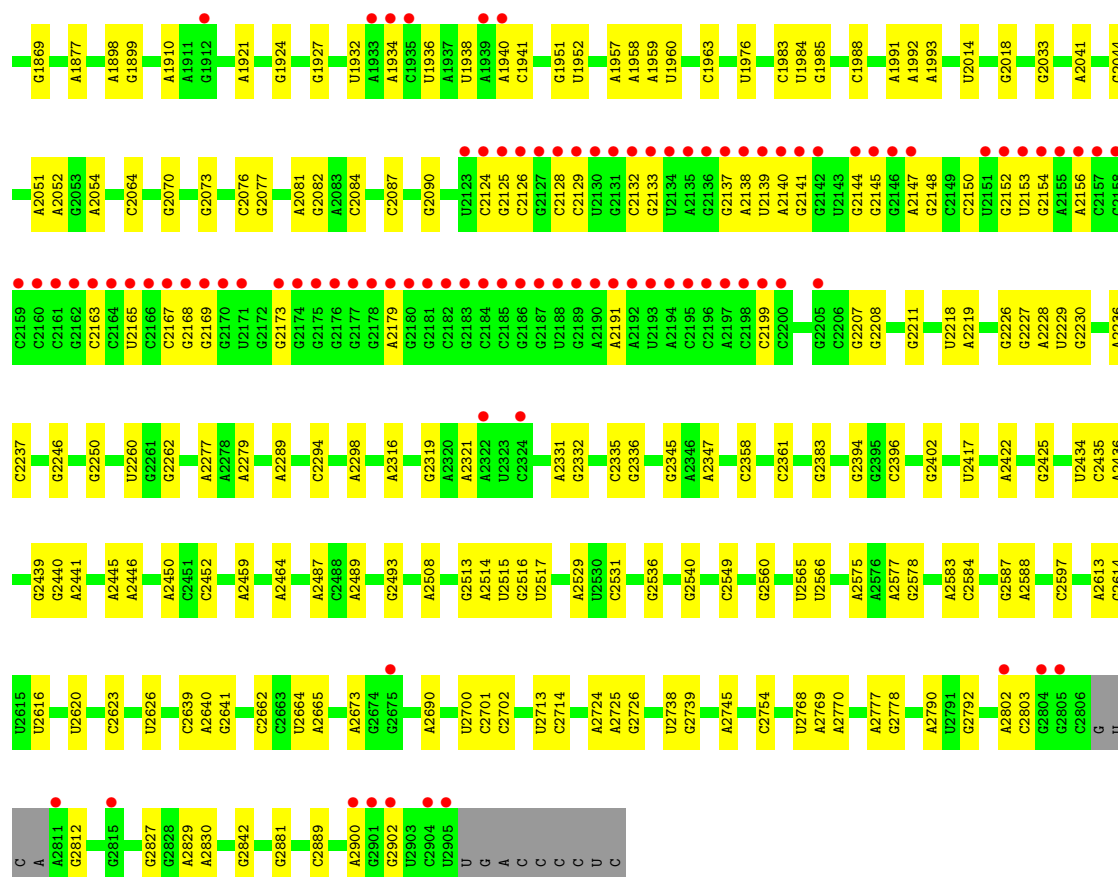
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	2T	4	Total 4	O 4	0	0
59	2U	5	Total 5	O 5	0	0
59	2V	3	Total 3	O 3	0	0
59	2W	4	Total 4	O 4	0	0
59	2X	5	Total 5	O 5	0	0
59	2Y	2	Total 2	O 2	0	0
59	20	5	Total 5	O 5	0	0
59	21	4	Total 4	O 4	0	0
59	22	1	Total 1	O 1	0	0
59	23	2	Total 2	O 2	0	0
59	25	1	Total 1	O 1	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

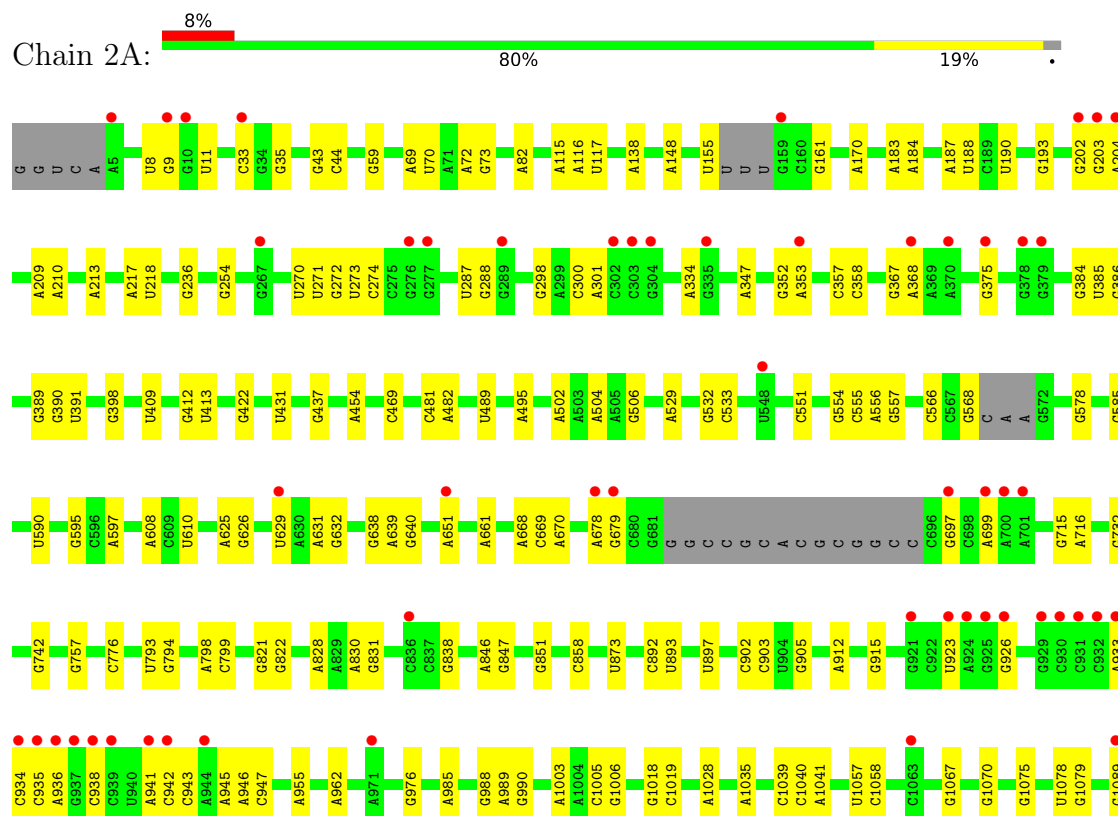
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

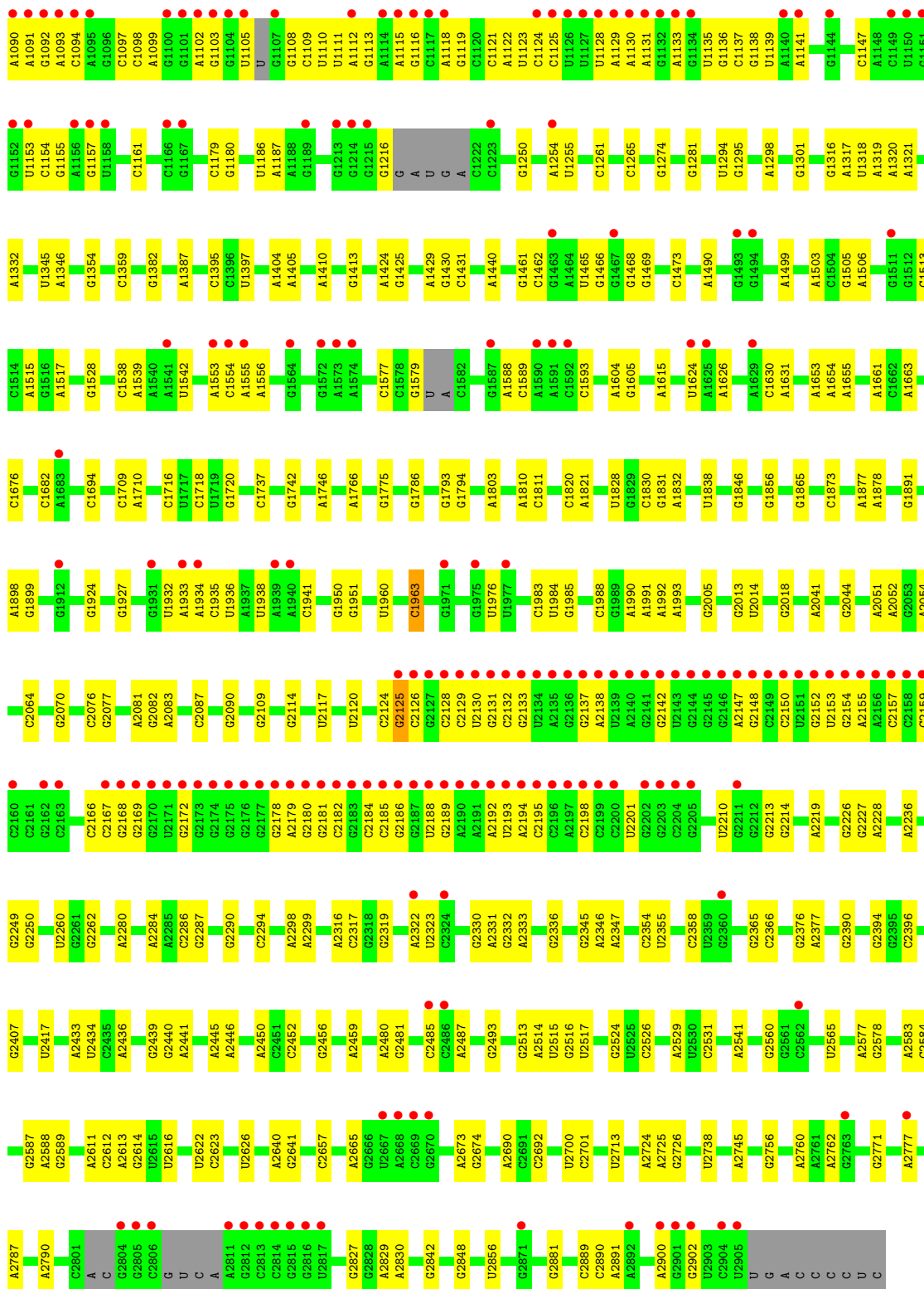
• Molecule 1: 23S Ribosomal RNA



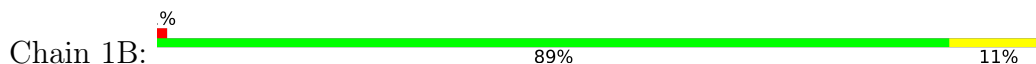


- Molecule 1: 23S Ribosomal RNA



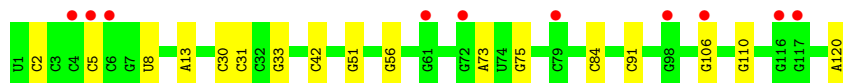
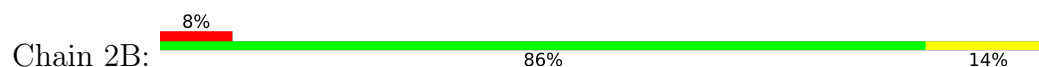


• Molecule 2: 5S Ribosomal RNA





- Molecule 2: 5S Ribosomal RNA



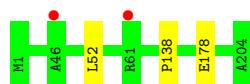
- Molecule 3: 50S ribosomal protein L2



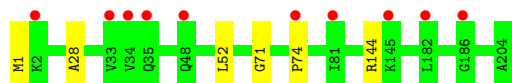
- Molecule 3: 50S ribosomal protein L2



- Molecule 4: 50S ribosomal protein L3



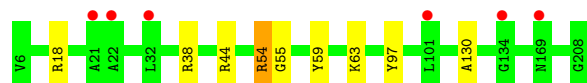
- Molecule 4: 50S ribosomal protein L3



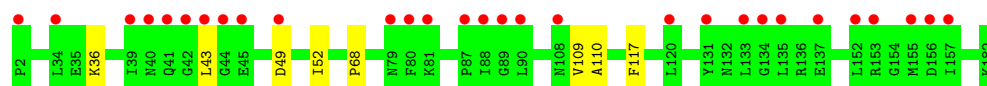
- Molecule 5: 50S ribosomal protein L4



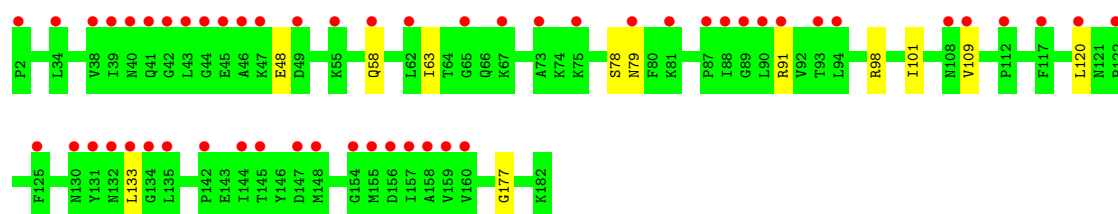
- Molecule 5: 50S ribosomal protein L4



- Molecule 6: 50S ribosomal protein L5



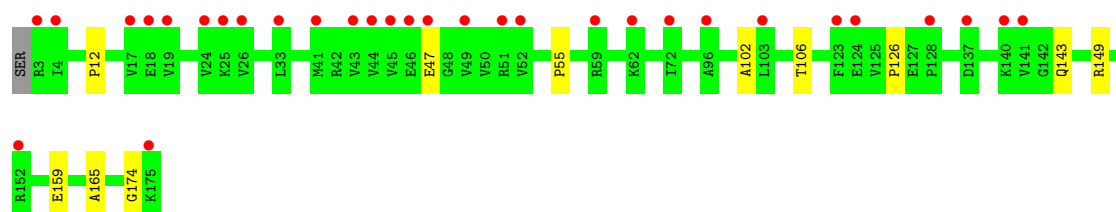
- Molecule 6: 50S ribosomal protein L5



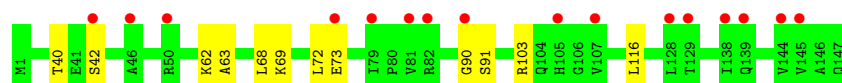
- Molecule 7: 50S ribosomal protein L6



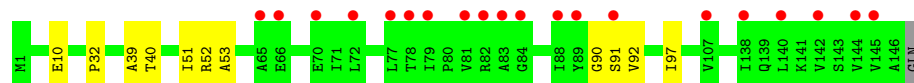
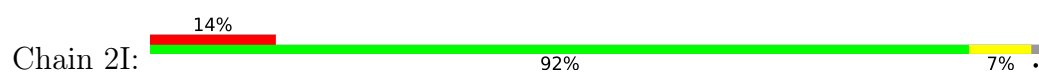
- Molecule 7: 50S ribosomal protein L6



- Molecule 8: 50S ribosomal protein L9



- Molecule 8: 50S ribosomal protein L9



- Molecule 9: 50S ribosomal protein L13



- Molecule 9: 50S ribosomal protein L13



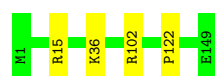
- Molecule 10: 50S ribosomal protein L14



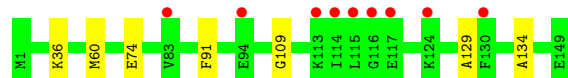
- Molecule 10: 50S ribosomal protein L14



- 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% •



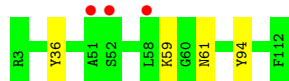
- Molecule 13: 50S ribosomal protein L17

Chain 2R:  92% 8% •



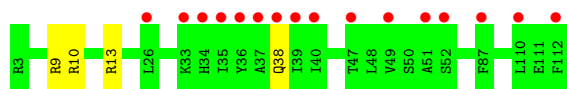
- Molecule 14: 50S ribosomal protein L18

Chain 1S:  96% 3% •



- Molecule 14: 50S ribosomal protein L18

Chain 2S:  96% 15% •

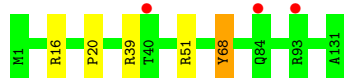


- Molecule 15: 50S ribosomal protein L19

Chain 1T:  92% 7% •



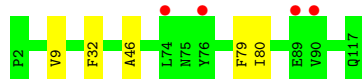
- Molecule 15: 50S ribosomal protein L19



- Molecule 16: 50S ribosomal protein L20



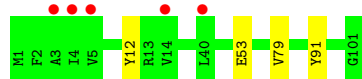
- Molecule 16: 50S ribosomal protein L20



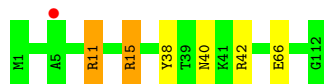
- Molecule 17: 50S ribosomal protein L21



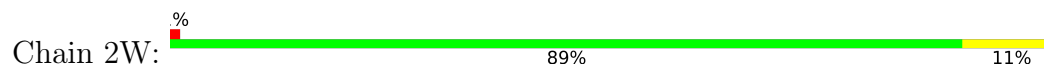
- Molecule 17: 50S ribosomal protein L21



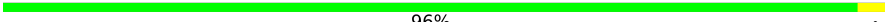
- Molecule 18: 50S ribosomal protein L22

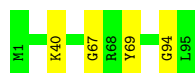


- Molecule 18: 50S ribosomal protein L22



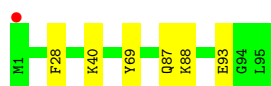
- Molecule 19: 50S ribosomal protein L23

Chain 1X:  96% .



- Molecule 19: 50S ribosomal protein L23

Chain 2X:  94% 6%



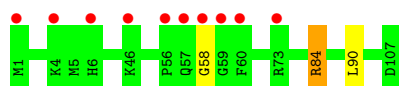
- Molecule 20: 50S ribosomal protein L24

Chain 1Y:  94% 6%



- Molecule 20: 50S ribosomal protein L24

Chain 2Y:  97% ..



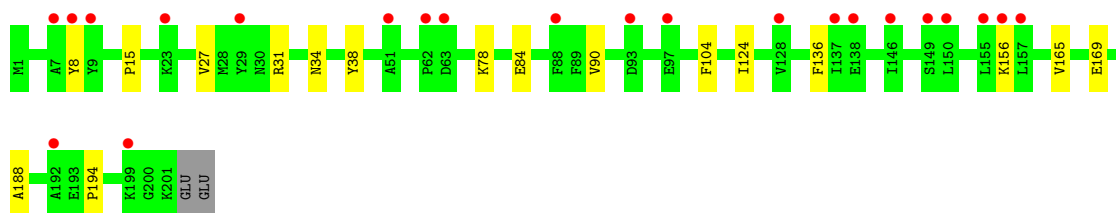
- Molecule 21: 50S ribosomal protein L25

Chain 1Z:  93% 7%



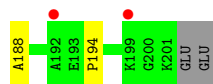
- Molecule 21: 50S ribosomal protein L25

Chain 2Z:  91% 8% .



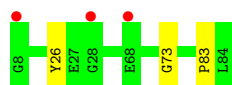
- Molecule 22: 50S ribosomal protein L27

Chain 10:  96% .





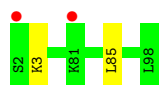
- Molecule 22: 50S ribosomal protein L27



- Molecule 23: 50S ribosomal protein L28



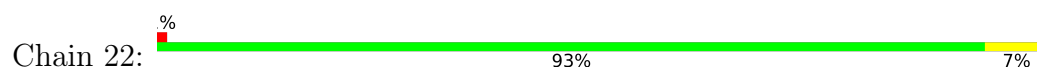
- Molecule 23: 50S ribosomal protein L28



- Molecule 24: 50S ribosomal protein L29



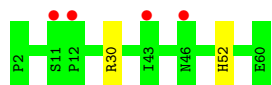
- Molecule 24: 50S ribosomal protein L29



- Molecule 25: 50S ribosomal protein L30



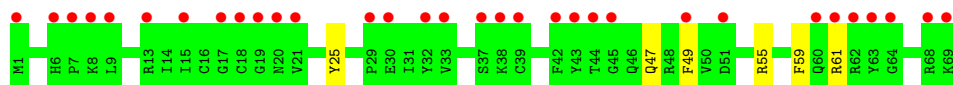
- Molecule 25: 50S ribosomal protein L30



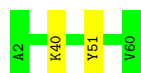
- Molecule 26: 50S ribosomal protein L31



- Molecule 26: 50S ribosomal protein L31



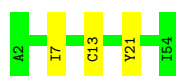
- Molecule 27: 50S ribosomal protein L32



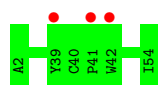
- Molecule 27: 50S ribosomal protein L32



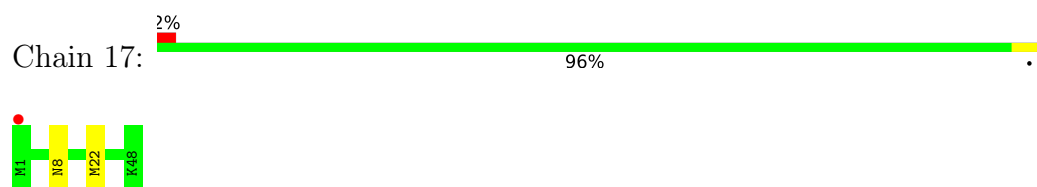
- Molecule 28: 50S ribosomal protein L33



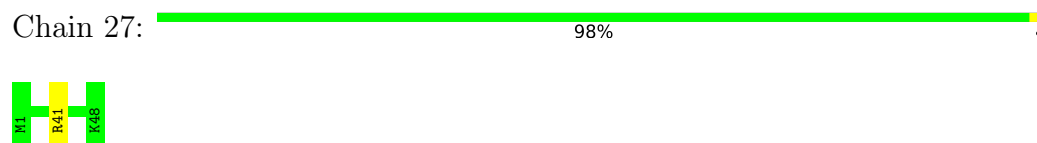
- Molecule 28: 50S ribosomal protein L33



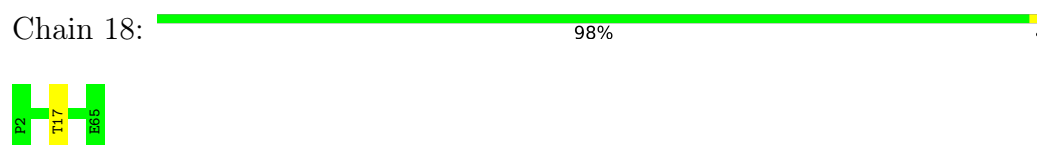
- Molecule 29: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L34



- Molecule 30: 50S ribosomal protein L35



- Molecule 30: 50S ribosomal protein L35



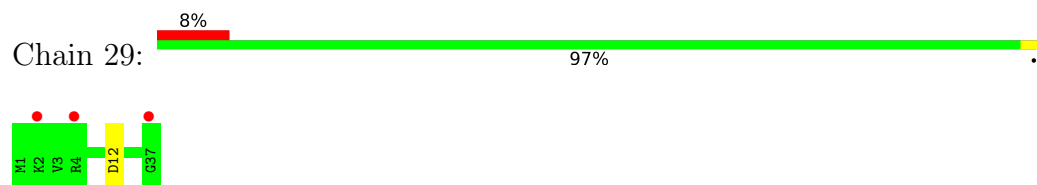
There are no outlier residues recorded for this chain.

- Molecule 31: 50S ribosomal protein L36

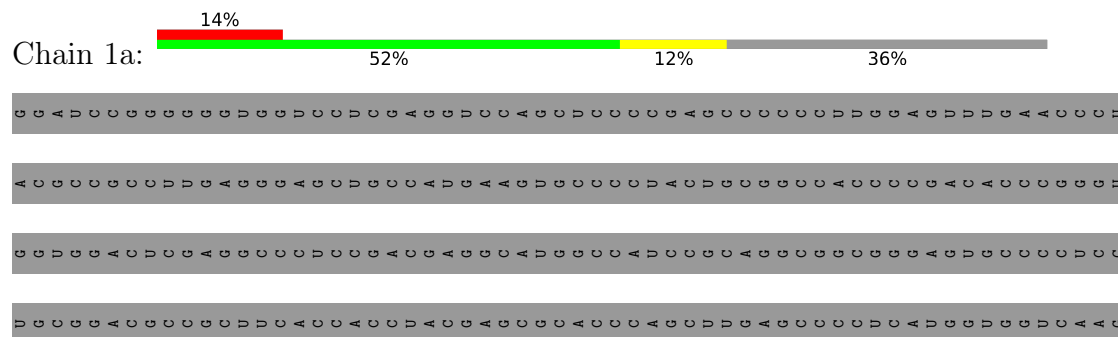


There are no outlier residues recorded for this chain.

- Molecule 31: 50S ribosomal protein L36

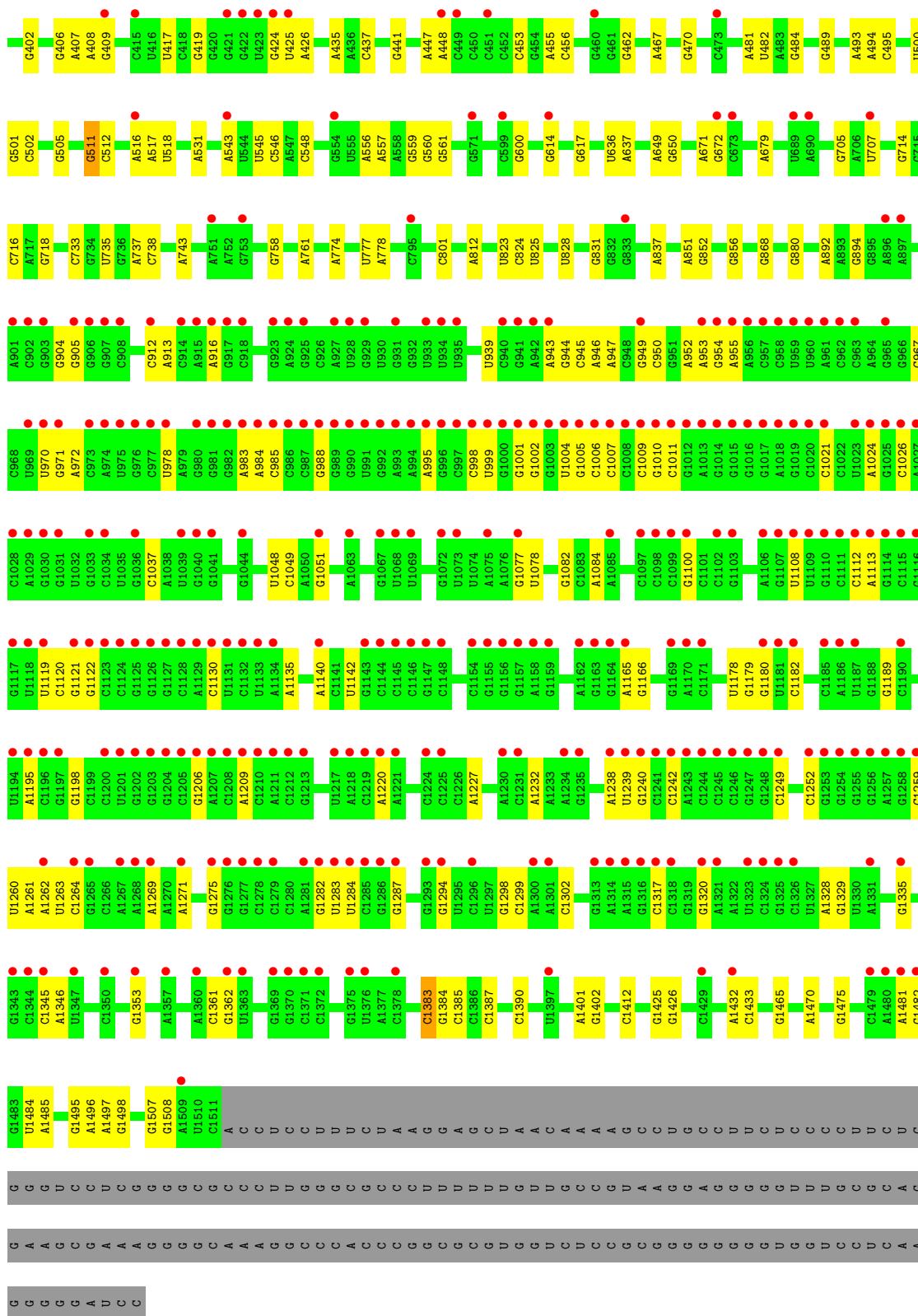


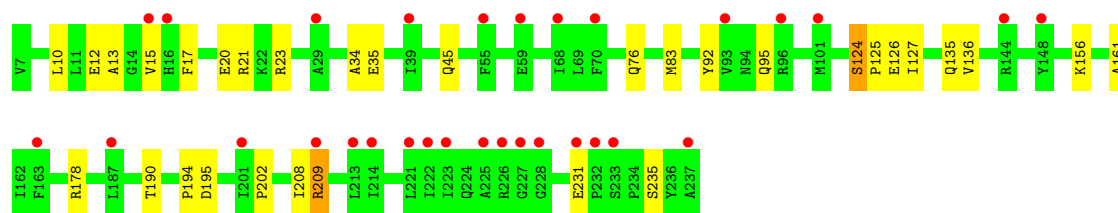
- Molecule 32: 16S Ribosomal RNA



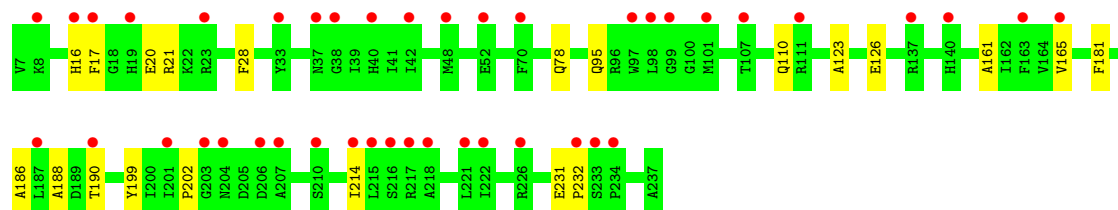
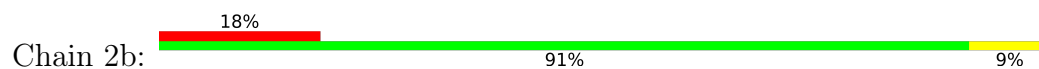




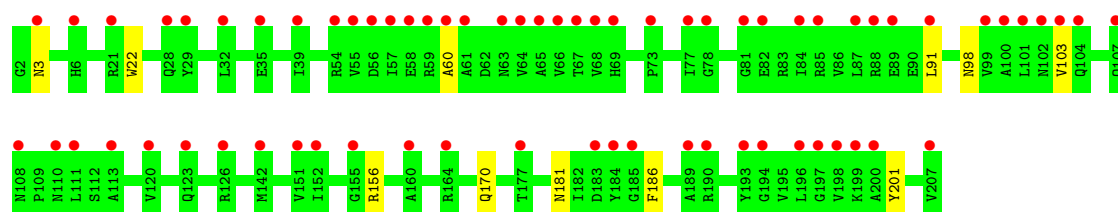




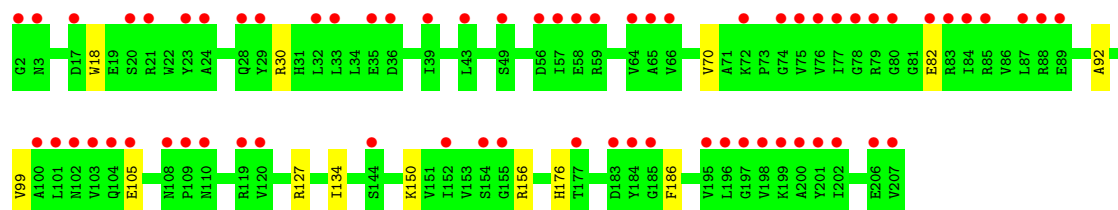
• Molecule 33: 30S ribosomal protein S2



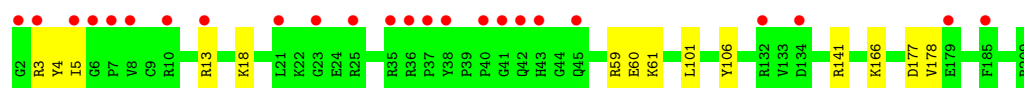
• Molecule 34: 30S ribosomal protein S3



• Molecule 34: 30S ribosomal protein S3

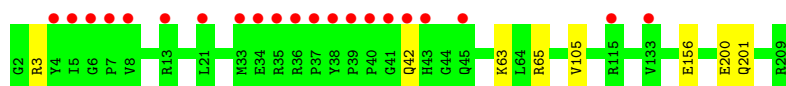


• Molecule 35: 30S ribosomal protein S4

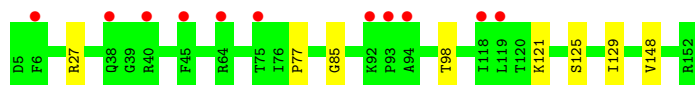


• Molecule 35: 30S ribosomal protein S4

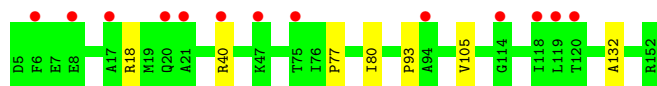




- Molecule 36: 30S ribosomal protein S5



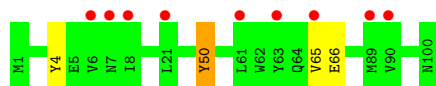
- Molecule 36: 30S ribosomal protein S5



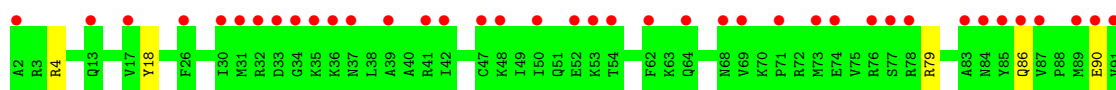
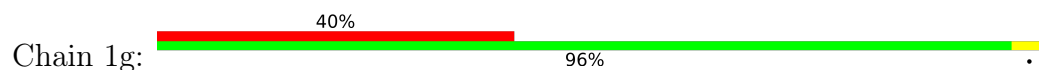
- Molecule 37: 30S ribosomal protein S6



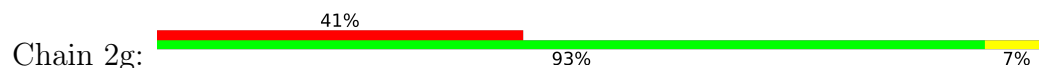
- Molecule 37: 30S ribosomal protein S6

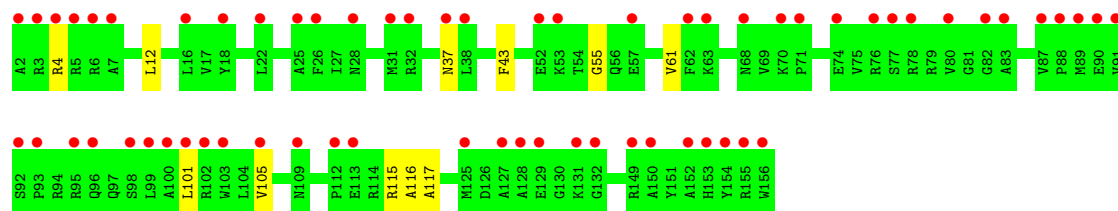


- Molecule 38: 30S ribosomal protein S7



- Molecule 38: 30S ribosomal protein S7

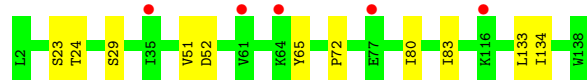
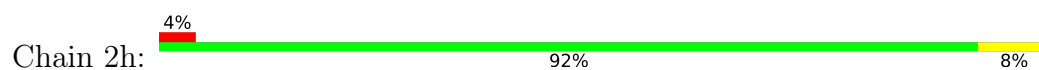




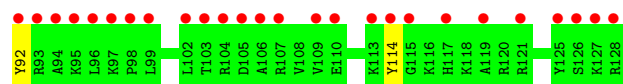
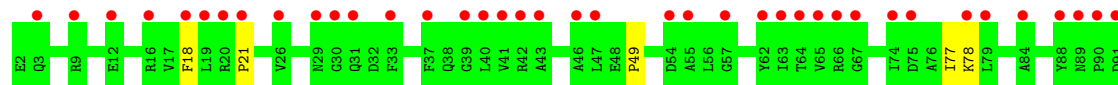
- Molecule 39: 30S ribosomal protein S8



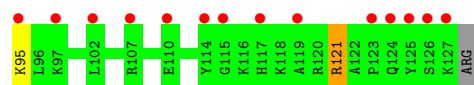
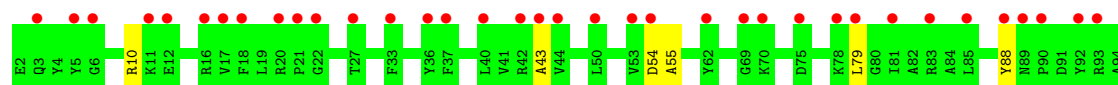
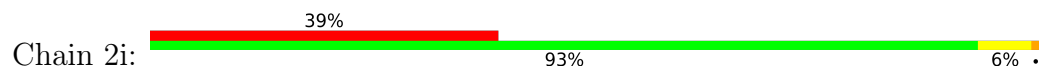
- Molecule 39: 30S ribosomal protein S8



- Molecule 40: 30S ribosomal protein S9

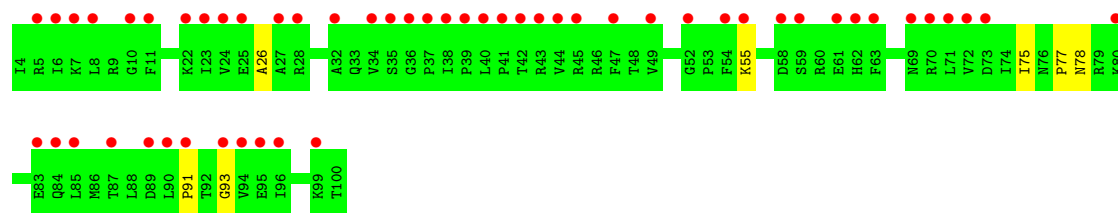


- Molecule 40: 30S ribosomal protein S9

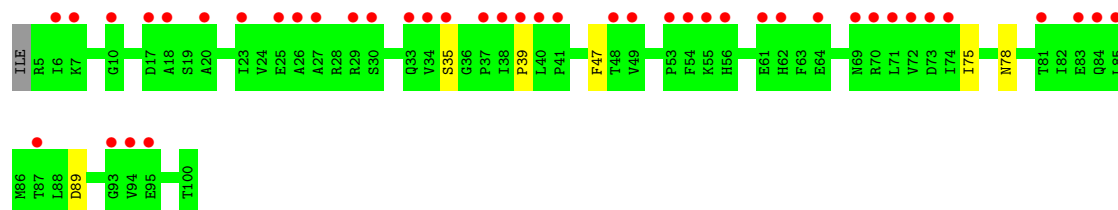
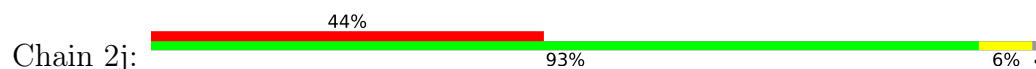


- Molecule 41: 30S ribosomal protein S10

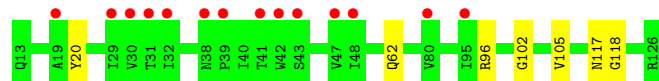




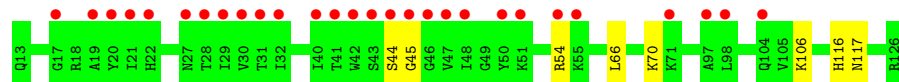
- Molecule 41: 30S ribosomal protein S10



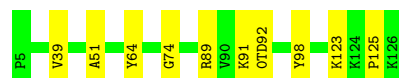
- Molecule 42: 30S ribosomal protein S11



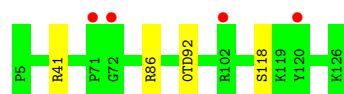
- Molecule 42: 30S ribosomal protein S11



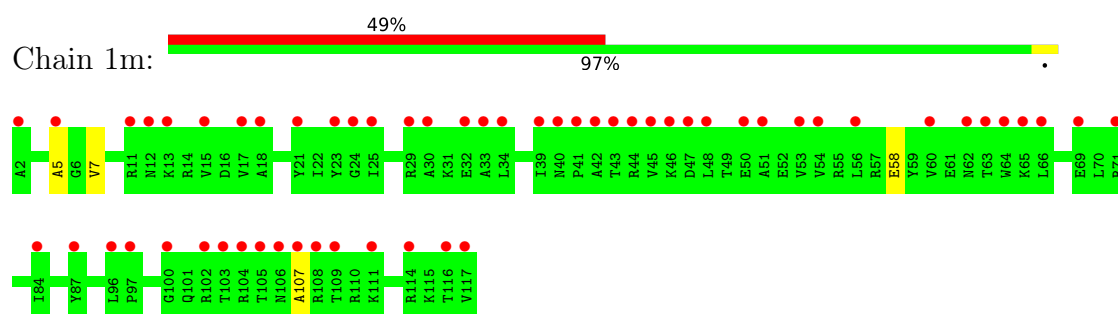
- Molecule 43: 30S ribosomal protein S12



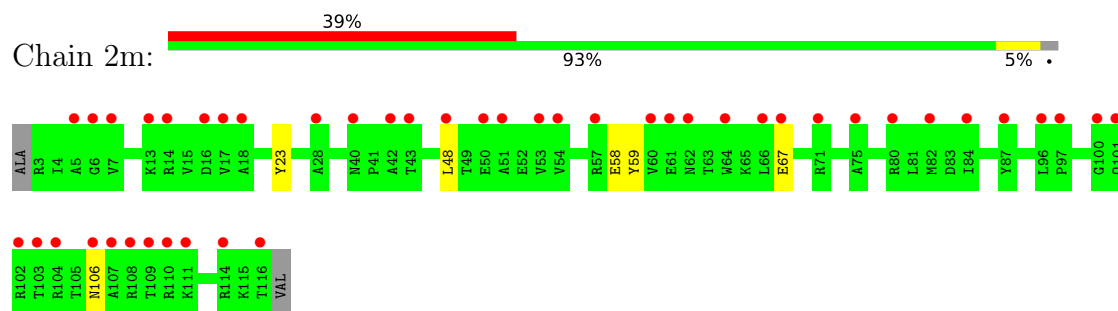
- Molecule 43: 30S ribosomal protein S12



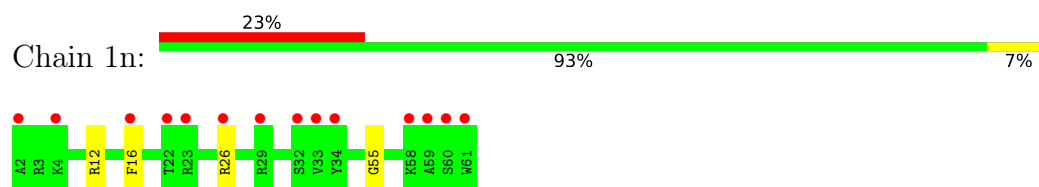
- Molecule 44: 30S ribosomal protein S13



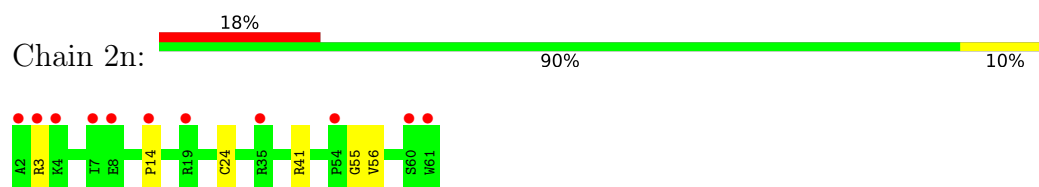
- Molecule 44: 30S ribosomal protein S13



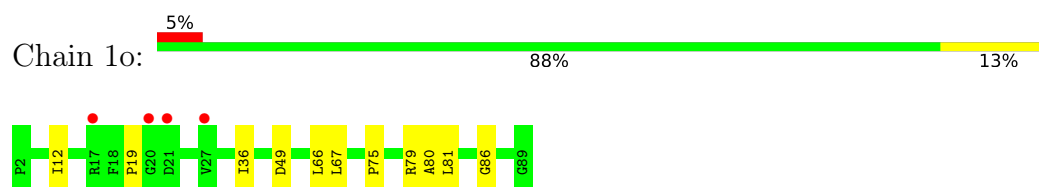
- Molecule 45: 30S ribosomal protein S14 type Z



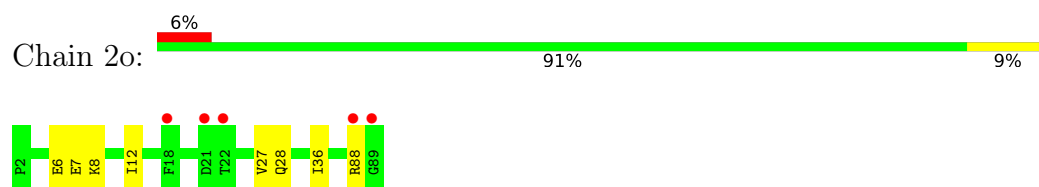
- Molecule 45: 30S ribosomal protein S14 type Z



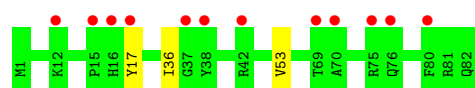
- Molecule 46: 30S ribosomal protein S15



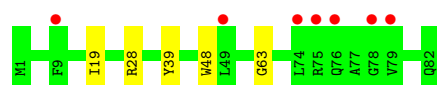
- Molecule 46: 30S ribosomal protein S15



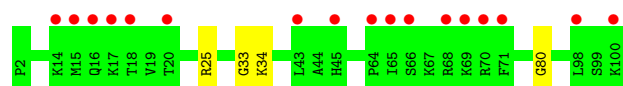
● Molecule 47: 30S ribosomal protein S16



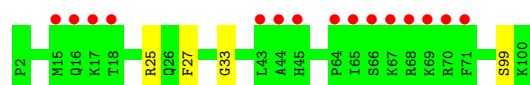
● Molecule 47: 30S ribosomal protein S16



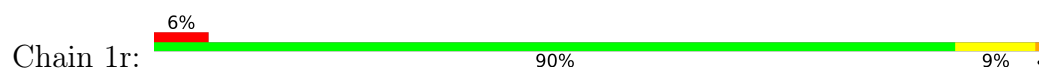
● Molecule 48: 30S ribosomal protein S17



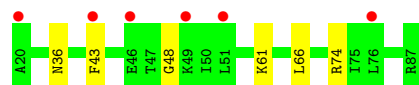
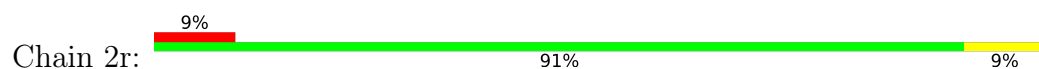
● Molecule 48: 30S ribosomal protein S17



● Molecule 49: 30S ribosomal protein S18

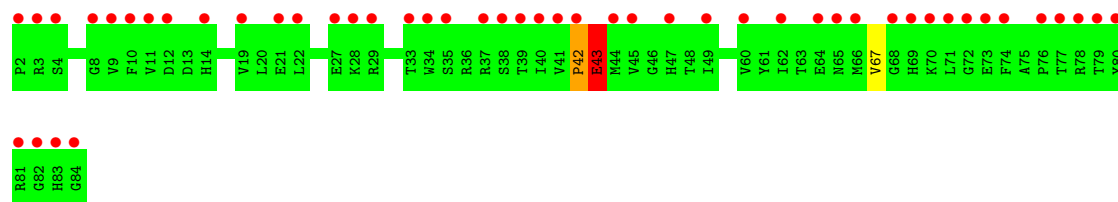


● Molecule 49: 30S ribosomal protein S18

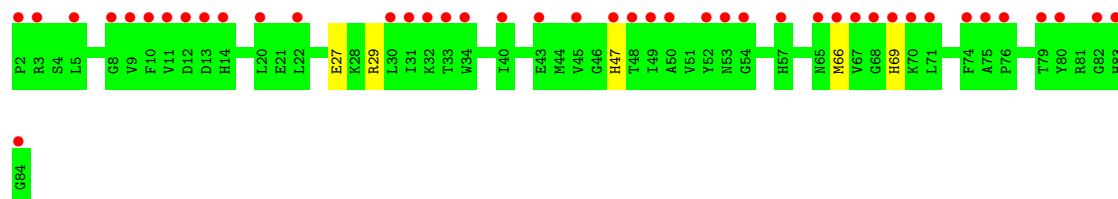


● Molecule 50: 30S ribosomal protein S19

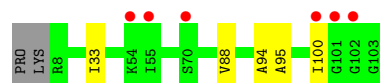




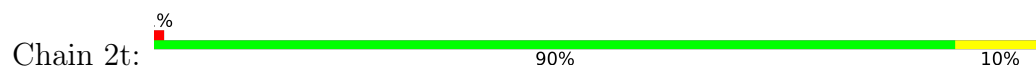
- Molecule 50: 30S ribosomal protein S19



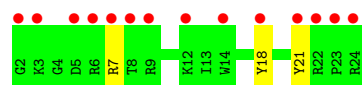
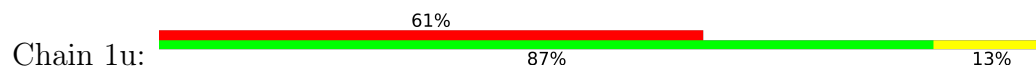
- Molecule 51: 30S ribosomal protein S20



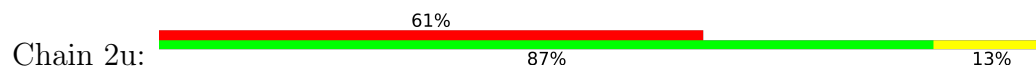
- Molecule 51: 30S ribosomal protein S20



- 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	74.6	Xtriage
Anisotropy	0.421	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 97.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, 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

All (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
50	1s	43	GLU	CG-CD	6.56	1.61	1.51
18	1W	11	ARG	CZ-NH2	6.46	1.41	1.33
50	1s	43	GLU	CD-OE1	-5.95	1.19	1.25

All (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
15	2T	16	ARG	NE-CZ-NH2	8.49	124.55	120.30
18	1W	11	ARG	NH1-CZ-NH2	7.70	127.87	119.40
42	2k	54	ARG	CG-CD-NE	7.53	127.61	111.80
35	1d	18	LYS	CD-CE-NZ	-7.51	94.42	111.70
50	1s	43	GLU	CG-CD-OE2	7.48	133.26	118.30
15	1T	74	ARG	NE-CZ-NH1	-7.41	116.59	120.30
18	1W	11	ARG	NE-CZ-NH1	7.22	123.91	120.30
50	1s	43	GLU	CB-CG-CD	-7.08	95.08	114.20
1	2A	1828	U	C4-C5-C6	7.03	123.92	119.70
42	2k	54	ARG	CB-CG-CD	-6.58	94.48	111.60
1	1A	715	G	C4-N9-C1'	6.39	134.81	126.50
50	1s	42	PRO	CA-C-N	6.34	131.14	117.20
1	1A	715	G	C8-N9-C1'	-6.28	118.84	127.00
1	2A	2125	G	C5-C6-O6	6.09	132.25	128.60
1	1A	1120	C	N1-C2-O2	6.08	122.55	118.90
34	2c	127	ARG	NE-CZ-NH1	6.07	123.34	120.30
1	2A	2125	G	N3-C2-N2	5.93	124.06	119.90
11	1P	102	ARG	NE-CZ-NH1	-5.87	117.36	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2D	274	ARG	CB-CG-CD	-5.82	96.48	111.60
33	1b	209	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	2A	2125	G	N1-C2-N2	-5.59	111.17	116.20
49	1r	29	PHE	CB-CG-CD2	-5.57	116.90	120.80
1	2A	1828	U	C5-C6-N1	-5.49	119.95	122.70
18	1W	11	ARG	CG-CD-NE	5.45	123.24	111.80
15	1T	74	ARG	NE-CZ-NH2	5.41	123.01	120.30
32	1a	1007	C	C2-N3-C4	5.38	122.59	119.90
32	2a	738	C	C2-N1-C1'	5.36	124.69	118.80
35	1d	141	ARG	NE-CZ-NH1	-5.31	117.64	120.30
3	1D	103	ARG	NE-CZ-NH1	-5.17	117.71	120.30
37	2f	50	TYR	CB-CG-CD2	-5.12	117.93	121.00
1	1A	1108	G	C5-C6-O6	5.09	131.66	128.60
42	2k	54	ARG	NE-CZ-NH2	5.08	122.84	120.30
42	2k	54	ARG	NE-CZ-NH1	-5.08	117.76	120.30
18	1W	11	ARG	CD-NE-CZ	5.02	130.63	123.60

There are no chirality outliers.

All (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
26	24	59	PHE	Peptide
3	2D	275	LYS	Peptide
42	2k	116	HIS	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/275 (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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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

All (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
7	1H	92	ILE
9	1N	23	LEU
12	1Q	59	ARG
12	1Q	78	PRO
15	1T	55	ASN
19	1X	40	LYS
19	1X	94	GLY
21	1Z	90	VAL
33	1b	10	LEU
33	1b	17	PHE
33	1b	21	ARG
33	1b	35	GLU
33	1b	124	SER
33	1b	125	PRO
33	1b	135	GLN
33	1b	136	VAL
33	1b	190	THR
33	1b	194	PRO
33	1b	195	ASP
35	1d	5	ILE
35	1d	59	ARG
35	1d	60	GLU
35	1d	61	LYS
35	1d	177	ASP

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Mol	Chain	Res	Type
36	1e	98	THR
36	1e	125	SER
39	1h	54	ASP
41	1j	77	PRO
43	1l	91	LYS
46	1o	80	ALA
49	1r	66	LEU
51	1t	95	ALA
4	2E	28	ALA
4	2E	52	LEU
5	2F	54	ARG
5	2F	130	ALA
6	2G	48	GLU
6	2G	78	SER
6	2G	133	LEU
7	2H	159	GLU
8	2I	10	GLU
8	2I	40	THR
9	2N	23	LEU
9	2N	30	ILE
16	2U	9	VAL
18	2W	15	ARG
18	2W	33	ARG
21	2Z	31	ARG
21	2Z	34	ASN
24	22	47	ASN
25	23	52	HIS
26	24	61	ARG
33	2b	16	HIS
33	2b	17	PHE
33	2b	95	GLN
33	2b	126	GLU
33	2b	181	PHE
33	2b	231	GLU
36	2e	105	VAL
37	2f	66	GLU
38	2g	4	ARG
38	2g	116	ALA
38	2g	117	ALA
39	2h	83	ILE
40	2i	10	ARG
40	2i	54	ASP

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Mol	Chain	Res	Type
41	2j	75	ILE
41	2j	89	ASP
42	2k	45	GLY
42	2k	117	ASN
44	2m	23	TYR
46	2o	6	GLU
46	2o	36	ILE
49	2r	36	ASN
49	2r	66	LEU
50	2s	27	GLU
51	2t	100	ILE
3	1D	31	LYS
3	1D	160	GLY
5	1F	17	ARG
5	1F	60	SER
5	1F	130	ALA
6	1G	43	LEU
6	1G	109	VAL
7	1H	100	GLY
8	1I	40	THR
8	1I	42	SER
8	1I	62	LYS
8	1I	103	ARG
10	1O	45	GLU
11	1P	15	ARG
12	1Q	13	GLN
12	1Q	51	ARG
12	1Q	110	THR
13	1R	58	GLY
15	1T	68	TYR
15	1T	127	ALA
17	1V	53	GLU
18	1W	15	ARG
18	1W	40	ASN
19	1X	67	GLY
20	1Y	51	VAL
21	1Z	11	GLU
21	1Z	120	ILE
25	13	13	ILE
26	14	44	THR
26	14	45	GLY
26	14	47	GLN

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Mol	Chain	Res	Type
26	14	60	GLN
28	16	13	CYS
33	1b	12	GLU
33	1b	45	GLN
33	1b	161	ALA
33	1b	208	ILE
33	1b	231	GLU
34	1c	3	ASN
34	1c	60	ALA
34	1c	98	ASN
34	1c	156	ARG
35	1d	3	ARG
35	1d	4	TYR
35	1d	101	LEU
35	1d	166	LYS
36	1e	85	GLY
37	1f	40	VAL
38	1g	4	ARG
41	1j	55	LYS
41	1j	93	GLY
42	1k	117	ASN
46	1o	49	ASP
46	1o	79	ARG
46	1o	81	LEU
48	1q	33	GLY
49	1r	62	GLU
49	1r	67	ALA
51	1t	94	ALA
52	1u	7	ARG
4	2E	144	ARG
6	2G	120	LEU
7	2H	47	GLU
8	2I	39	ALA
10	2O	29	ASN
10	2O	45	GLU
12	2Q	59	ARG
13	2R	58	GLY
14	2S	9	ARG
17	2V	53	GLU
18	2W	71	VAL
18	2W	98	LYS
18	2W	111	HIS

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Mol	Chain	Res	Type
20	2Y	58	GLY
20	2Y	84	ARG
21	2Z	78	LYS
21	2Z	156	LYS
21	2Z	169	GLU
21	2Z	188	ALA
23	21	3	LYS
24	22	32	LEU
26	24	49	PHE
31	29	12	ASP
33	2b	165	VAL
33	2b	188	ALA
33	2b	214	ILE
34	2c	99	VAL
35	2d	105	VAL
37	2f	65	VAL
38	2g	55	GLY
39	2h	24	THR
39	2h	133	LEU
39	2h	134	ILE
40	2i	121	ARG
42	2k	106	LYS
43	2l	41	ARG
44	2m	48	LEU
44	2m	67	GLU
45	2n	3	ARG
45	2n	56	VAL
46	2o	8	LYS
46	2o	28	GLN
47	2p	19	ILE
47	2p	48	TRP
48	2q	33	GLY
49	2r	74	ARG
51	2t	9	ASN
51	2t	63	ILE
52	2u	13	ILE
3	1D	14	ARG
3	1D	241	PRO
4	1E	178	GLU
5	1F	207	GLY
6	1G	117	PHE
7	1H	82	GLY

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Mol	Chain	Res	Type
7	1H	96	ALA
8	1I	72	LEU
8	1I	116	LEU
13	1R	8	ARG
14	1S	61	ASN
20	1Y	78	ALA
20	1Y	90	LEU
21	1Z	66	SER
21	1Z	183	LEU
22	10	48	GLY
23	11	3	LYS
24	12	50	ILE
24	12	69	ARG
26	14	49	PHE
30	18	17	THR
33	1b	13	ALA
33	1b	34	ALA
33	1b	126	GLU
33	1b	209	ARG
36	1e	121	LYS
37	1f	62	TRP
39	1h	51	VAL
39	1h	77	GLU
42	1k	96	ARG
42	1k	102	GLY
43	1l	51	ALA
43	1l	64	TYR
43	1l	123	LYS
43	1l	125	PRO
44	1m	5	ALA
44	1m	58	GLU
46	1o	67	LEU
49	1r	34	TYR
49	1r	52	PRO
49	1r	60	ALA
3	2D	118	VAL
4	2E	71	GLY
6	2G	79	ASN
6	2G	91	ARG
7	2H	55	PRO
7	2H	102	ALA
7	2H	106	THR

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Mol	Chain	Res	Type
7	2H	126	PRO
7	2H	143	GLN
8	2I	53	ALA
8	2I	97	ILE
9	2N	28	THR
9	2N	29	LYS
9	2N	81	GLY
9	2N	111	PRO
10	2O	26	LYS
11	2P	36	LYS
11	2P	109	GLY
12	2Q	14	ARG
13	2R	3	HIS
13	2R	14	SER
13	2R	15	SER
13	2R	86	ARG
14	2S	10	ARG
14	2S	38	GLN
15	2T	68	TYR
16	2U	46	ALA
16	2U	79	PHE
18	2W	40	ASN
18	2W	59	VAL
19	2X	87	GLN
19	2X	88	LYS
19	2X	93	GLU
23	2I	85	LEU
24	22	69	ARG
33	2b	21	ARG
33	2b	110	GLN
33	2b	123	ALA
33	2b	186	ALA
33	2b	232	PRO
34	2c	18	TRP
34	2c	82	GLU
34	2c	156	ARG
35	2d	42	GLN
35	2d	63	LYS
35	2d	201	GLN
36	2e	40	ARG
38	2g	12	LEU
38	2g	61	VAL

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Mol	Chain	Res	Type
38	2g	101	LEU
39	2h	23	SER
40	2i	43	ALA
41	2j	35	SER
41	2j	78	ASN
43	2l	118	SER
44	2m	58	GLU
44	2m	59	TYR
44	2m	106	ASN
45	2n	14	PRO
45	2n	24	CYS
45	2n	41	ARG
46	2o	7	GLU
46	2o	12	ILE
46	2o	27	VAL
47	2p	28	ARG
47	2p	63	GLY
48	2q	99	SER
49	2r	61	LYS
50	2s	29	ARG
50	2s	66	MET
51	2t	10	LEU
51	2t	102	GLY
3	1D	218	ARG
3	1D	236	GLY
4	1E	52	LEU
4	1E	138	PRO
8	1I	63	ALA
8	1I	73	GLU
10	1O	5	GLN
15	1T	128	GLU
18	1W	66	GLU
21	1Z	34	ASN
21	1Z	40	ASP
21	1Z	41	LEU
21	1Z	119	GLU
21	1Z	136	PHE
22	10	9	SER
29	17	8	ASN
33	1b	23	ARG
33	1b	76	GLN
33	1b	83	MET

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Mol	Chain	Res	Type
33	1b	235	SER
36	1e	27	ARG
38	1g	90	GLU
40	1i	78	LYS
41	1j	91	PRO
42	1k	62	GLN
45	1n	26	ARG
46	1o	12	ILE
46	1o	19	PRO
46	1o	66	LEU
3	2D	53	PHE
3	2D	156	ALA
5	2F	63	LYS
7	2H	12	PRO
8	2I	92	VAL
10	2O	89	ASN
11	2P	60	MET
12	2Q	40	ALA
13	2R	27	SER
13	2R	45	ARG
18	2W	11	ARG
18	2W	58	ALA
19	2X	40	LYS
21	2Z	84	GLU
24	22	33	MET
33	2b	161	ALA
33	2b	190	THR
34	2c	150	LYS
34	2c	176	HIS
35	2d	200	GLU
36	2e	132	ALA
39	2h	29	SER
39	2h	52	ASP
40	2i	55	ALA
40	2i	95	LYS
42	2k	66	LEU
43	2l	86	ARG
50	2s	69	HIS
51	2t	27	LYS
51	2t	89	ARG
3	1D	203	ASN
3	1D	263	ARG

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Mol	Chain	Res	Type
6	1G	36	LYS
6	1G	68	PRO
7	1H	110	SER
8	1I	69	LYS
8	1I	90	GLY
9	1N	112	LEU
10	1O	54	GLU
12	1Q	40	ALA
14	1S	59	LYS
17	1V	43	GLU
21	1Z	65	GLN
21	1Z	93	ASP
24	12	26	ARG
33	1b	20	GLU
33	1b	95	GLN
33	1b	178	ARG
34	1c	22	TRP
34	1c	91	LEU
34	1c	170	GLN
34	1c	181	ASN
35	1d	13	ARG
36	1e	148	VAL
37	1f	19	LEU
38	1g	93	PRO
39	1h	35	ILE
39	1h	70	GLN
41	1j	78	ASN
43	1l	74	GLY
46	1o	36	ILE
3	2D	241	PRO
5	2F	59	TYR
6	2G	58	GLN
6	2G	63	ILE
6	2G	98	ARG
7	2H	165	ALA
7	2H	174	GLY
8	2I	52	ARG
9	2N	98	VAL
11	2P	134	ALA
13	2R	13	HIS
15	2T	20	PRO
16	2U	80	ILE

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Mol	Chain	Res	Type
20	2Y	90	LEU
21	2Z	165	VAL
26	24	47	GLN
33	2b	20	GLU
33	2b	78	GLN
33	2b	202	PRO
34	2c	30	ARG
34	2c	92	ALA
38	2g	43	PHE
39	2h	80	ILE
40	2i	88	TYR
42	2k	70	LYS
46	2o	88	ARG
49	2r	48	GLY
50	2s	47	HIS
51	2t	8	ARG
51	2t	74	LYS
3	1D	45	ASN
3	1D	132	PRO
5	1F	61	GLY
8	1I	68	LEU
11	1P	36	LYS
12	1Q	50	ALA
13	1R	86	ARG
14	1S	94	TYR
15	1T	36	GLU
15	1T	120	ARG
22	10	83	PRO
29	17	22	MET
33	1b	15	VAL
33	1b	127	ILE
38	1g	86	GLN
39	1h	13	ILE
40	1i	21	PRO
41	1j	26	ALA
44	1m	107	ALA
45	1n	55	GLY
46	1o	86	GLY
47	1p	53	VAL
48	1q	34	LYS
48	1q	80	GLY
51	1t	33	ILE

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Mol	Chain	Res	Type
4	2E	74	PRO
8	2I	51	ILE
10	2O	115	VAL
11	2P	74	GLU
11	2P	129	ALA
13	2R	39	PRO
17	2V	79	VAL
18	2W	14	PRO
18	2W	80	PRO
21	2Z	27	VAL
26	24	55	ARG
34	2c	70	VAL
34	2c	105	GLU
35	2d	156	GLU
36	2e	77	PRO
36	2e	80	ILE
36	2e	93	PRO
40	2i	79	LEU
42	2k	44	SER
48	2q	27	PHE
51	2t	33	ILE
11	1P	122	PRO
20	1Y	15	VAL
28	16	7	ILE
33	1b	202	PRO
36	1e	77	PRO
39	1h	83	ILE
41	1j	75	ILE
42	1k	105	VAL
42	1k	118	GLY
47	1p	36	ILE
50	1s	67	VAL
8	2I	90	GLY
21	2Z	124	ILE
21	2Z	194	PRO
38	2g	105	VAL
39	2h	51	VAL
17	1V	79	VAL
40	1i	49	PRO
5	2F	55	GLY
6	2G	101	ILE
10	2O	119	PRO

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Mol	Chain	Res	Type
18	2W	21	VAL
34	2c	134	ILE
9	1N	30	ILE
12	1Q	109	VAL
34	1c	103	VAL
36	1e	129	ILE
6	2G	109	VAL
6	2G	177	GLY
21	2Z	15	PRO
22	20	83	PRO
39	2h	72	PRO
45	2n	55	GLY
13	1R	39	PRO
35	1d	178	VAL
39	1h	86	ILE
44	1m	7	VAL
46	1o	75	PRO
51	1t	88	VAL
51	1t	100	ILE
3	2D	244	ARG
8	2I	32	PRO
21	2Z	90	VAL
23	11	74	VAL
40	1i	77	ILE
43	1l	39	VAL
22	20	73	GLY
41	2j	39	PRO
52	2u	23	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	2E	164/165 (99%)	163 (99%)	1 (1%)	86	94
5	1F	160/161 (99%)	157 (98%)	3 (2%)	57	80
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	1Y	86/88 (98%)	84 (98%)	2 (2%)	50	75
20	2Y	86/88 (98%)	85 (99%)	1 (1%)	71	87
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	2e	114/114 (100%)	113 (99%)	1 (1%)	78	90
37	1f	85/90 (94%)	85 (100%)	0	100	100
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	1u	18/18 (100%)	16 (89%)	2 (11%)	6	23
52	2u	18/18 (100%)	17 (94%)	1 (6%)	21	50
All	All	9364/9696 (97%)	9258 (99%)	106 (1%)	73	88

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	9	TYR
5	1F	38	ARG
5	1F	44	ARG
5	1F	54	ARG
7	1H	95	ARG
9	1N	115	ARG
10	1O	79	PHE
12	1Q	29	PHE
12	1Q	51	ARG
12	1Q	65	PHE
14	1S	36	TYR
15	1T	14	TYR
15	1T	41	ARG
15	1T	74	ARG
15	1T	115	ARG
16	1U	79	PHE
17	1V	91	TYR
18	1W	11	ARG
18	1W	15	ARG
18	1W	38	TYR
18	1W	42	ARG
19	1X	69	TYR
20	1Y	20	TYR
20	1Y	43	ASN
21	1Z	8	TYR
21	1Z	38	TYR
26	14	32	TYR
26	14	67	TYR
27	15	40	LYS
27	15	51	TYR
28	16	21	TYR
33	1b	92	TYR
33	1b	156	LYS
34	1c	186	PHE

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Mol	Chain	Res	Type
34	1c	201	TYR
35	1d	106	TYR
38	1g	18	TYR
38	1g	79	ARG
39	1h	65	TYR
40	1i	18	PHE
40	1i	92	TYR
40	1i	114	TYR
42	1k	20	TYR
43	1l	89	ARG
43	1l	98	TYR
45	1n	12	ARG
45	1n	16	PHE
47	1p	17	TYR
48	1q	25	ARG
49	1r	29	PHE
50	1s	43	GLU
52	1u	18	TYR
52	1u	21	TYR
3	2D	9	TYR
3	2D	84	TYR
4	2E	1	MET
5	2F	18	ARG
5	2F	38	ARG
5	2F	44	ARG
5	2F	54	ARG
5	2F	97	TYR
7	2H	149	ARG
9	2N	4	TYR
9	2N	12	ARG
10	2O	99	PHE
11	2P	91	PHE
12	2Q	6	ARG
12	2Q	93	TYR
12	2Q	130	LYS
12	2Q	137	TYR
14	2S	13	ARG
15	2T	39	ARG
15	2T	51	ARG
15	2T	68	TYR
16	2U	32	PHE
17	2V	12	TYR

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Mol	Chain	Res	Type
17	2V	91	TYR
19	2X	28	PHE
19	2X	69	TYR
20	2Y	84	ARG
21	2Z	8	TYR
21	2Z	38	TYR
21	2Z	104	PHE
21	2Z	136	PHE
22	20	26	TYR
24	22	65	ASN
25	23	30	ARG
26	24	25	TYR
29	27	41	ARG
33	2b	28	PHE
33	2b	199	TYR
34	2c	186	PHE
35	2d	3	ARG
35	2d	65	ARG
36	2e	18	ARG
37	2f	4	TYR
37	2f	50	TYR
38	2g	37	ASN
38	2g	115	ARG
39	2h	65	TYR
40	2i	121	ARG
41	2j	47	PHE
47	2p	39	TYR
48	2q	25	ARG
49	2r	43	PHE
52	2u	21	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (128) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	87	ASN
3	1D	115	GLN
3	1D	116	GLN
4	1E	48	GLN
4	1E	159	HIS
4	1E	180	ASN
6	1G	40	ASN
7	1H	74	ASN

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Mol	Chain	Res	Type
8	1I	104	GLN
8	1I	105	HIS
10	1O	5	GLN
11	1P	27	HIS
12	1Q	57	HIS
12	1Q	123	HIS
13	1R	23	ASN
13	1R	24	GLN
13	1R	50	HIS
13	1R	71	GLN
14	1S	68	GLN
15	1T	58	ASN
16	1U	117	GLN
18	1W	34	ASN
18	1W	60	ASN
18	1W	102	HIS
19	1X	31	HIS
19	1X	41	ASN
20	1Y	92	ASN
21	1Z	34	ASN
23	1I	56	GLN
24	1J	65	ASN
25	1K	52	HIS
27	1L	23	HIS
28	1M	20	ASN
28	1M	29	ASN
31	1N	20	HIS
33	1b	19	HIS
33	1b	40	HIS
33	1b	95	GLN
33	1b	113	HIS
33	1b	212	GLN
34	1c	6	HIS
34	1c	37	GLN
34	1c	69	HIS
34	1c	139	GLN
35	1d	119	GLN
35	1d	123	HIS
35	1d	125	HIS
36	1e	20	GLN
37	1f	100	ASN
38	1g	37	ASN

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Mol	Chain	Res	Type
38	1g	122	HIS
38	1g	153	HIS
39	1h	15	ASN
40	1i	3	GLN
40	1i	31	GLN
40	1i	38	GLN
41	1j	21	GLN
41	1j	56	HIS
41	1j	84	GLN
43	1l	49	ASN
46	1o	28	GLN
46	1o	37	ASN
48	1q	16	GLN
50	1s	23	ASN
50	1s	69	HIS
50	1s	83	HIS
51	1t	73	HIS
51	1t	75	ASN
3	2D	115	GLN
3	2D	116	GLN
3	2D	143	HIS
3	2D	253	GLN
4	2E	48	GLN
4	2E	137	HIS
4	2E	169	ASN
5	2F	40	GLN
5	2F	75	HIS
6	2G	108	ASN
6	2G	132	ASN
7	2H	74	ASN
8	2I	105	HIS
11	2P	27	HIS
11	2P	35	HIS
12	2Q	13	GLN
12	2Q	57	HIS
13	2R	13	HIS
15	2T	58	ASN
15	2T	123	GLN
16	2U	94	ASN
18	2W	40	ASN
18	2W	57	ASN
18	2W	60	ASN

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Mol	Chain	Res	Type
21	2Z	55	HIS
21	2Z	85	HIS
26	24	46	GLN
27	25	23	HIS
28	26	20	ASN
28	26	29	ASN
31	29	36	GLN
33	2b	16	HIS
33	2b	113	HIS
33	2b	212	GLN
34	2c	6	HIS
35	2d	119	GLN
35	2d	125	HIS
35	2d	201	GLN
36	2e	78	HIS
37	2f	64	GLN
37	2f	73	ASN
38	2g	109	ASN
38	2g	148	ASN
39	2h	82	HIS
40	2i	3	GLN
41	2j	21	GLN
43	2l	49	ASN
44	2m	77	ASN
44	2m	92	HIS
44	2m	101	GLN
45	2n	49	HIS
46	2o	28	GLN
46	2o	37	ASN
46	2o	62	GLN
48	2q	94	ASN
49	2r	63	GLN
50	2s	23	ASN
50	2s	69	HIS
50	2s	83	HIS
51	2t	16	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	485 (16%)	22 (0%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
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%)

All (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
1	1A	59	G
1	1A	69	A
1	1A	72	A
1	1A	73	G
1	1A	98	G
1	1A	115	A
1	1A	116	A
1	1A	117	U
1	1A	120	G
1	1A	122	G
1	1A	138	A
1	1A	161	G
1	1A	170	A
1	1A	174	G
1	1A	175	G
1	1A	184	A
1	1A	187	A
1	1A	193	G
1	1A	203	G
1	1A	204	A
1	1A	209	A
1	1A	210	A
1	1A	217	A
1	1A	218	U
1	1A	229	A
1	1A	236	G
1	1A	237	C

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Mol	Chain	Res	Type
1	1A	254	G
1	1A	268	G
1	1A	270	U
1	1A	271	U
1	1A	272	G
1	1A	273	U
1	1A	274	C
1	1A	287	U
1	1A	288	G
1	1A	294	C
1	1A	295	U
1	1A	298	G
1	1A	302	C
1	1A	334	A
1	1A	348	G
1	1A	353	A
1	1A	354	A
1	1A	361	G
1	1A	375	G
1	1A	386	G
1	1A	388	G
1	1A	398	G
1	1A	412	G
1	1A	415	G
1	1A	416	A
1	1A	422	G
1	1A	431	U
1	1A	432	G
1	1A	433	G
1	1A	437	G
1	1A	454	A
1	1A	473	U
1	1A	474	A
1	1A	481	C
1	1A	482	A
1	1A	490	G
1	1A	498	G
1	1A	505	A
1	1A	506	G
1	1A	529	A
1	1A	532	G
1	1A	533	C

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Mol	Chain	Res	Type
1	1A	537	A
1	1A	552	A
1	1A	553	A
1	1A	554	G
1	1A	555	C
1	1A	556	A
1	1A	557	G
1	1A	560	A
1	1A	568	G
1	1A	572	G
1	1A	573	G
1	1A	578	G
1	1A	585	G
1	1A	590	U
1	1A	595	G
1	1A	604	G
1	1A	625	A
1	1A	626	G
1	1A	629	U
1	1A	638	G
1	1A	640	G
1	1A	641	G
1	1A	643	G
1	1A	651	A
1	1A	659	C
1	1A	661	A
1	1A	669	C
1	1A	670	A
1	1A	696	C
1	1A	697	G
1	1A	714	G
1	1A	715	G
1	1A	716	A
1	1A	719	C
1	1A	728	G
1	1A	732	G
1	1A	763	G
1	1A	776	C
1	1A	794	G
1	1A	811	G
1	1A	817	G
1	1A	820	A

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Mol	Chain	Res	Type
1	1A	821	G
1	1A	822	G
1	1A	825	U
1	1A	828	A
1	1A	830	A
1	1A	831	G
1	1A	836	C
1	1A	838	G
1	1A	851	G
1	1A	857	U
1	1A	858	C
1	1A	873	U
1	1A	874	U
1	1A	877	G
1	1A	902	C
1	1A	905	G
1	1A	912	A
1	1A	925	G
1	1A	931	C
1	1A	932	C
1	1A	934	C
1	1A	935	C
1	1A	936	A
1	1A	941	A
1	1A	952	U
1	1A	955	A
1	1A	976	G
1	1A	989	A
1	1A	990	G
1	1A	997	A
1	1A	1003	A
1	1A	1005	C
1	1A	1018	G
1	1A	1019	C
1	1A	1020	G
1	1A	1028	A
1	1A	1034	G
1	1A	1035	A
1	1A	1039	C
1	1A	1040	C
1	1A	1041	A
1	1A	1050	C

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Mol	Chain	Res	Type
1	1A	1057	U
1	1A	1058	C
1	1A	1067	G
1	1A	1068	U
1	1A	1069	G
1	1A	1070	G
1	1A	1071	U
1	1A	1078	U
1	1A	1084	G
1	1A	1085	C
1	1A	1088	C
1	1A	1090	A
1	1A	1091	A
1	1A	1092	G
1	1A	1096	G
1	1A	1098	C
1	1A	1099	A
1	1A	1106	U
1	1A	1107	G
1	1A	1110	U
1	1A	1113	G
1	1A	1115	A
1	1A	1118	A
1	1A	1119	G
1	1A	1120	C
1	1A	1121	C
1	1A	1122	A
1	1A	1123	U
1	1A	1124	C
1	1A	1128	U
1	1A	1132	G
1	1A	1133	A
1	1A	1135	U
1	1A	1137	C
1	1A	1141	A
1	1A	1149	C
1	1A	1154	C
1	1A	1155	G
1	1A	1157	G
1	1A	1172	A
1	1A	1174	A
1	1A	1175	U

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Mol	Chain	Res	Type
1	1A	1177	A
1	1A	1179	C
1	1A	1180	G
1	1A	1186	U
1	1A	1216	G
1	1A	1217	G
1	1A	1218	A
1	1A	1219	U
1	1A	1220	G
1	1A	1221	A
1	1A	1222	C
1	1A	1254	A
1	1A	1255	U
1	1A	1262	C
1	1A	1281	G
1	1A	1295	G
1	1A	1298	A
1	1A	1301	G
1	1A	1316	G
1	1A	1317	A
1	1A	1318	U
1	1A	1321	A
1	1A	1329	A
1	1A	1345	U
1	1A	1346	A
1	1A	1368	U
1	1A	1390	C
1	1A	1393	G
1	1A	1395	C
1	1A	1397	U
1	1A	1404	A
1	1A	1410	A
1	1A	1423	A
1	1A	1424	A
1	1A	1429	A
1	1A	1430	G
1	1A	1431	C
1	1A	1461	G
1	1A	1462	C
1	1A	1465	U
1	1A	1466	G
1	1A	1472	A

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Mol	Chain	Res	Type
1	1A	1473	C
1	1A	1478	U
1	1A	1490	A
1	1A	1500	U
1	1A	1501	G
1	1A	1507	G
1	1A	1513	C
1	1A	1515	A
1	1A	1517	A
1	1A	1528	G
1	1A	1538	C
1	1A	1540	A
1	1A	1551	C
1	1A	1554	C
1	1A	1555	A
1	1A	1577	C
1	1A	1578	C
1	1A	1588	A
1	1A	1589	C
1	1A	1592	C
1	1A	1604	A
1	1A	1615	A
1	1A	1624	U
1	1A	1625	A
1	1A	1626	A
1	1A	1630	C
1	1A	1631	A
1	1A	1647	U
1	1A	1653	A
1	1A	1654	A
1	1A	1655	A
1	1A	1661	A
1	1A	1663	A
1	1A	1685	U
1	1A	1694	C
1	1A	1700	A
1	1A	1710	A
1	1A	1720	G
1	1A	1740	C
1	1A	1742	G
1	1A	1746	A
1	1A	1747	A

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Mol	Chain	Res	Type
1	1A	1766	A
1	1A	1767	U
1	1A	1775	G
1	1A	1778	G
1	1A	1792	A
1	1A	1793	G
1	1A	1794	G
1	1A	1803	A
1	1A	1810	A
1	1A	1821	A
1	1A	1830	C
1	1A	1831	G
1	1A	1845	A
1	1A	1846	G
1	1A	1849	A
1	1A	1857	C
1	1A	1863	U
1	1A	1869	G
1	1A	1877	A
1	1A	1898	A
1	1A	1899	G
1	1A	1910	A
1	1A	1921	A
1	1A	1924	G
1	1A	1927	G
1	1A	1934	A
1	1A	1940	A
1	1A	1951	G
1	1A	1952	U
1	1A	1957	A
1	1A	1958	A
1	1A	1959	A
1	1A	1976	U
1	1A	1984	U
1	1A	1985	G
1	1A	1988	C
1	1A	1991	A
1	1A	1992	A
1	1A	1993	A
1	1A	2014	U
1	1A	2018	G
1	1A	2033	G

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Mol	Chain	Res	Type
1	1A	2041	A
1	1A	2044	G
1	1A	2051	A
1	1A	2052	A
1	1A	2054	A
1	1A	2064	C
1	1A	2070	G
1	1A	2073	G
1	1A	2076	C
1	1A	2077	G
1	1A	2081	A
1	1A	2082	G
1	1A	2084	C
1	1A	2087	C
1	1A	2090	G
1	1A	2124	C
1	1A	2125	G
1	1A	2126	C
1	1A	2128	C
1	1A	2129	C
1	1A	2133	G
1	1A	2137	G
1	1A	2138	A
1	1A	2139	U
1	1A	2140	A
1	1A	2141	G
1	1A	2144	G
1	1A	2145	G
1	1A	2147	A
1	1A	2148	G
1	1A	2150	C
1	1A	2152	G
1	1A	2153	U
1	1A	2154	G
1	1A	2156	A
1	1A	2163	C
1	1A	2165	U
1	1A	2167	C
1	1A	2168	G
1	1A	2169	G
1	1A	2173	G
1	1A	2179	A

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Mol	Chain	Res	Type
1	1A	2191	A
1	1A	2199	C
1	1A	2207	G
1	1A	2208	G
1	1A	2211	G
1	1A	2219	A
1	1A	2226	G
1	1A	2227	G
1	1A	2228	A
1	1A	2229	U
1	1A	2230	G
1	1A	2236	A
1	1A	2237	C
1	1A	2246	G
1	1A	2250	G
1	1A	2260	U
1	1A	2277	A
1	1A	2279	A
1	1A	2289	A
1	1A	2294	C
1	1A	2298	A
1	1A	2316	A
1	1A	2319	G
1	1A	2321	A
1	1A	2331	A
1	1A	2332	G
1	1A	2335	C
1	1A	2336	G
1	1A	2345	G
1	1A	2347	A
1	1A	2358	C
1	1A	2361	C
1	1A	2383	G
1	1A	2394	G
1	1A	2396	C
1	1A	2402	G
1	1A	2417	U
1	1A	2422	A
1	1A	2425	G
1	1A	2434	U
1	1A	2435	C
1	1A	2436	A

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Mol	Chain	Res	Type
1	1A	2439	G
1	1A	2440	G
1	1A	2441	A
1	1A	2445	A
1	1A	2446	A
1	1A	2450	A
1	1A	2452	C
1	1A	2459	A
1	1A	2464	A
1	1A	2487	A
1	1A	2489	A
1	1A	2493	G
1	1A	2508	A
1	1A	2513	G
1	1A	2515	U
1	1A	2516	G
1	1A	2517	U
1	1A	2529	A
1	1A	2531	C
1	1A	2536	G
1	1A	2540	G
1	1A	2549	C
1	1A	2560	G
1	1A	2565	U
1	1A	2566	U
1	1A	2575	A
1	1A	2577	A
1	1A	2578	G
1	1A	2583	A
1	1A	2584	C
1	1A	2587	G
1	1A	2588	A
1	1A	2597	C
1	1A	2613	A
1	1A	2614	G
1	1A	2620	U
1	1A	2623	C
1	1A	2626	U
1	1A	2639	C
1	1A	2640	A
1	1A	2641	G
1	1A	2662	C

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Mol	Chain	Res	Type
1	1A	2664	U
1	1A	2665	A
1	1A	2673	A
1	1A	2690	A
1	1A	2700	U
1	1A	2701	C
1	1A	2702	C
1	1A	2713	U
1	1A	2714	C
1	1A	2724	A
1	1A	2725	A
1	1A	2726	G
1	1A	2738	U
1	1A	2739	G
1	1A	2745	A
1	1A	2754	C
1	1A	2769	A
1	1A	2770	A
1	1A	2777	A
1	1A	2778	G
1	1A	2790	A
1	1A	2792	G
1	1A	2802	A
1	1A	2803	C
1	1A	2812	G
1	1A	2827	G
1	1A	2829	A
1	1A	2830	A
1	1A	2842	G
1	1A	2881	G
1	1A	2889	C
1	1A	2900	A
1	1A	2902	G
2	1B	7	G
2	1B	13	A
2	1B	31	C
2	1B	41	U
2	1B	52	A
2	1B	56	G
2	1B	64	C
2	1B	73	A
2	1B	80	U

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Mol	Chain	Res	Type
2	1B	91	C
2	1B	101	G
2	1B	106	G
2	1B	110	G
32	1a	10	G
32	1a	23	G
32	1a	33	A
32	1a	40	G
32	1a	48	C
32	1a	49	C
32	1a	51	A
32	1a	52	A
32	1a	62	G
32	1a	76	G
32	1a	78	G
32	1a	95	A
32	1a	110	A
32	1a	115	C
32	1a	124	G
32	1a	126	C
32	1a	139	G
32	1a	156	A
32	1a	158	C
32	1a	168	U
32	1a	169	C
32	1a	177	U
32	1a	190	U
32	1a	191	G
32	1a	202	A
32	1a	208	C
32	1a	210	U
32	1a	211	U
32	1a	212	G
32	1a	239	A
32	1a	241	C
32	1a	243	G
32	1a	247	G
32	1a	259	A
32	1a	262	G
32	1a	263	C
32	1a	285	G
32	1a	294	A

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Mol	Chain	Res	Type
32	1a	324	C
32	1a	325	A
32	1a	326	C
32	1a	328	G
32	1a	344	G
32	1a	348	C
32	1a	349	A
32	1a	350	G
32	1a	363	U
32	1a	368	C
32	1a	369	A
32	1a	380	G
32	1a	383	U
32	1a	393	A
32	1a	394	C
32	1a	401	U
32	1a	402	G
32	1a	408	A
32	1a	409	G
32	1a	419	G
32	1a	420	G
32	1a	425	U
32	1a	426	A
32	1a	435	A
32	1a	437	C
32	1a	447	A
32	1a	455	A
32	1a	456	C
32	1a	457	G
32	1a	463	A
32	1a	469	G
32	1a	470	G
32	1a	481	A
32	1a	482	U
32	1a	489	G
32	1a	493	A
32	1a	494	A
32	1a	495	C
32	1a	496	U
32	1a	498	C
32	1a	502	C
32	1a	504	A

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Mol	Chain	Res	Type
32	1a	516	A
32	1a	517	A
32	1a	531	A
32	1a	543	A
32	1a	545	U
32	1a	546	C
32	1a	553	C
32	1a	556	A
32	1a	557	A
32	1a	559	G
32	1a	560	G
32	1a	561	G
32	1a	580	C
32	1a	582	U
32	1a	603	U
32	1a	604	C
32	1a	614	G
32	1a	615	G
32	1a	616	A
32	1a	637	A
32	1a	645	G
32	1a	646	G
32	1a	649	A
32	1a	650	G
32	1a	671	A
32	1a	672	G
32	1a	677	G
32	1a	691	C
32	1a	706	A
32	1a	707	U
32	1a	744	G
32	1a	750	A
32	1a	761	A
32	1a	773	U
32	1a	774	A
32	1a	776	A
32	1a	777	U
32	1a	778	A
32	1a	794	C
32	1a	801	C
32	1a	812	A
32	1a	813	G

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Mol	Chain	Res	Type
32	1a	820	G
32	1a	824	C
32	1a	825	U
32	1a	829	G
32	1a	837	A
32	1a	850	A
32	1a	851	A
32	1a	880	G
32	1a	892	A
32	1a	894	G
32	1a	904	G
32	1a	905	G
32	1a	906	G
32	1a	912	C
32	1a	913	A
32	1a	938	U
32	1a	939	U
32	1a	944	M2G
32	1a	946	A
32	1a	947	A
32	1a	949	G
32	1a	950	C
32	1a	952	A
32	1a	953	A
32	1a	954	G
32	1a	955	A
32	1a	960	U
32	1a	963	C
32	1a	970	U
32	1a	971	G
32	1a	972	A
32	1a	976	G
32	1a	982	G
32	1a	983	A
32	1a	984	A
32	1a	985	C
32	1a	996	G
32	1a	999	U
32	1a	1001	G
32	1a	1002	G
32	1a	1003	G
32	1a	1004	U

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Mol	Chain	Res	Type
32	1a	1005	G
32	1a	1006	C
32	1a	1007	C
32	1a	1008	C
32	1a	1010	G
32	1a	1011	C
32	1a	1012	G
32	1a	1015	G
32	1a	1016	G
32	1a	1019	G
32	1a	1020	C
32	1a	1025	G
32	1a	1026	C
32	1a	1027	A
32	1a	1036	G
32	1a	1048	U
32	1a	1049	C
32	1a	1051	G
32	1a	1053	U
32	1a	1063	A
32	1a	1064	G
32	1a	1072	G
32	1a	1077	G
32	1a	1078	U
32	1a	1084	A
32	1a	1106	A
32	1a	1108	U
32	1a	1113	A
32	1a	1115	C
32	1a	1117	G
32	1a	1119	U
32	1a	1120	C
32	1a	1121	G
32	1a	1122	G
32	1a	1123	C
32	1a	1135	A
32	1a	1142	U
32	1a	1143	G
32	1a	1150	A
32	1a	1161	A
32	1a	1165	A
32	1a	1166	G

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Mol	Chain	Res	Type
32	1a	1175	G
32	1a	1176	U
32	1a	1178	U
32	1a	1179	G
32	1a	1183	A
32	1a	1184	G
32	1a	1190	C
32	1a	1194	U
32	1a	1195	A
32	1a	1196	C
32	1a	1206	G
32	1a	1207	A
32	1a	1208	C
32	1a	1209	A
32	1a	1211	A
32	1a	1218	A
32	1a	1220	A
32	1a	1226	C
32	1a	1236	C
32	1a	1238	A
32	1a	1239	U
32	1a	1240	G
32	1a	1243	A
32	1a	1260	U
32	1a	1262	A
32	1a	1268	A
32	1a	1269	A
32	1a	1272	G
32	1a	1279	C
32	1a	1281	A
32	1a	1284	U
32	1a	1300	A
32	1a	1301	A
32	1a	1302	C
32	1a	1314	A
32	1a	1316	G
32	1a	1318	C
32	1a	1328	A
32	1a	1329	G
32	1a	1335	G
32	1a	1341	C
32	1a	1345	C

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Mol	Chain	Res	Type
32	1a	1346	A
32	1a	1347	U
32	1a	1353	G
32	1a	1362	G
32	1a	1364	U
32	1a	1381	A
32	1a	1382	C
32	1a	1383	5MC
32	1a	1384	G
32	1a	1402	G
32	1a	1405	G
32	1a	1424	G
32	1a	1425	G
32	1a	1426	G
32	1a	1427	A
32	1a	1432	A
32	1a	1433	C
32	1a	1434	G
32	1a	1435	G
32	1a	1465	G
32	1a	1470	A
32	1a	1471	A
32	1a	1481	A
32	1a	1482	G
32	1a	1483	G
32	1a	1484	U
32	1a	1495	G
32	1a	1498	G
32	1a	1507	G
32	1a	1508	G
1	2A	9	G
1	2A	11	U
1	2A	33	C
1	2A	35	G
1	2A	43	G
1	2A	44	C
1	2A	59	G
1	2A	69	A
1	2A	70	U
1	2A	72	A
1	2A	73	G
1	2A	82	A

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Mol	Chain	Res	Type
1	2A	115	A
1	2A	116	A
1	2A	117	U
1	2A	138	A
1	2A	148	A
1	2A	155	U
1	2A	161	G
1	2A	170	A
1	2A	184	A
1	2A	187	A
1	2A	188	U
1	2A	190	U
1	2A	193	G
1	2A	203	G
1	2A	204	A
1	2A	209	A
1	2A	210	A
1	2A	213	A
1	2A	217	A
1	2A	218	U
1	2A	236	G
1	2A	254	G
1	2A	270	U
1	2A	271	U
1	2A	273	U
1	2A	274	C
1	2A	287	U
1	2A	288	G
1	2A	298	G
1	2A	300	C
1	2A	301	A
1	2A	334	A
1	2A	347	A
1	2A	352	G
1	2A	353	A
1	2A	358	C
1	2A	368	A
1	2A	375	G
1	2A	385	U
1	2A	386	G
1	2A	389	G
1	2A	390	G

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Mol	Chain	Res	Type
1	2A	391	U
1	2A	398	G
1	2A	409	U
1	2A	412	G
1	2A	413	U
1	2A	422	G
1	2A	431	U
1	2A	437	G
1	2A	454	A
1	2A	469	C
1	2A	481	C
1	2A	482	A
1	2A	489	U
1	2A	495	A
1	2A	502	A
1	2A	504	A
1	2A	506	G
1	2A	529	A
1	2A	532	G
1	2A	533	C
1	2A	551	C
1	2A	554	G
1	2A	555	C
1	2A	556	A
1	2A	557	G
1	2A	566	C
1	2A	568	G
1	2A	578	G
1	2A	585	G
1	2A	590	U
1	2A	595	G
1	2A	597	A
1	2A	608	A
1	2A	610	U
1	2A	625	A
1	2A	626	G
1	2A	629	U
1	2A	631	A
1	2A	632	G
1	2A	638	G
1	2A	639	A
1	2A	640	G

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Mol	Chain	Res	Type
1	2A	651	A
1	2A	661	A
1	2A	669	C
1	2A	670	A
1	2A	678	A
1	2A	679	G
1	2A	697	G
1	2A	699	A
1	2A	715	G
1	2A	716	A
1	2A	732	G
1	2A	757	G
1	2A	776	C
1	2A	793	U
1	2A	794	G
1	2A	798	A
1	2A	799	C
1	2A	821	G
1	2A	822	G
1	2A	828	A
1	2A	830	A
1	2A	831	G
1	2A	838	G
1	2A	847	G
1	2A	851	G
1	2A	858	C
1	2A	873	U
1	2A	892	C
1	2A	893	U
1	2A	897	U
1	2A	903	C
1	2A	905	G
1	2A	912	A
1	2A	915	G
1	2A	923	U
1	2A	926	G
1	2A	933	A
1	2A	934	C
1	2A	935	C
1	2A	936	A
1	2A	938	C
1	2A	941	A

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Mol	Chain	Res	Type
1	2A	942	C
1	2A	943	C
1	2A	945	A
1	2A	946	A
1	2A	947	C
1	2A	955	A
1	2A	962	A
1	2A	976	G
1	2A	985	A
1	2A	988	G
1	2A	989	A
1	2A	990	G
1	2A	1003	A
1	2A	1005	C
1	2A	1006	G
1	2A	1018	G
1	2A	1019	C
1	2A	1028	A
1	2A	1035	A
1	2A	1040	C
1	2A	1041	A
1	2A	1057	U
1	2A	1058	C
1	2A	1067	G
1	2A	1070	G
1	2A	1075	G
1	2A	1078	U
1	2A	1079	G
1	2A	1089	G
1	2A	1090	A
1	2A	1091	A
1	2A	1092	G
1	2A	1093	A
1	2A	1094	C
1	2A	1097	C
1	2A	1098	C
1	2A	1099	A
1	2A	1102	A
1	2A	1103	G
1	2A	1105	U
1	2A	1108	G
1	2A	1109	C

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Mol	Chain	Res	Type
1	2A	1110	U
1	2A	1111	U
1	2A	1112	A
1	2A	1113	G
1	2A	1115	A
1	2A	1116	G
1	2A	1118	A
1	2A	1119	G
1	2A	1121	C
1	2A	1122	A
1	2A	1123	U
1	2A	1124	C
1	2A	1125	C
1	2A	1128	U
1	2A	1129	A
1	2A	1130	A
1	2A	1131	A
1	2A	1133	A
1	2A	1135	U
1	2A	1136	G
1	2A	1137	C
1	2A	1138	G
1	2A	1139	U
1	2A	1141	A
1	2A	1147	C
1	2A	1153	U
1	2A	1154	C
1	2A	1155	G
1	2A	1157	G
1	2A	1161	C
1	2A	1179	C
1	2A	1180	G
1	2A	1186	U
1	2A	1187	A
1	2A	1216	G
1	2A	1250	G
1	2A	1255	U
1	2A	1261	C
1	2A	1265	C
1	2A	1274	G
1	2A	1281	G
1	2A	1294	U

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Mol	Chain	Res	Type
1	2A	1295	G
1	2A	1298	A
1	2A	1301	G
1	2A	1316	G
1	2A	1317	A
1	2A	1318	U
1	2A	1319	A
1	2A	1321	A
1	2A	1332	A
1	2A	1345	U
1	2A	1346	A
1	2A	1354	G
1	2A	1359	C
1	2A	1382	G
1	2A	1387	A
1	2A	1395	C
1	2A	1397	U
1	2A	1404	A
1	2A	1405	A
1	2A	1410	A
1	2A	1413	G
1	2A	1424	A
1	2A	1425	G
1	2A	1429	A
1	2A	1430	G
1	2A	1431	C
1	2A	1440	A
1	2A	1461	G
1	2A	1462	C
1	2A	1465	U
1	2A	1466	G
1	2A	1468	G
1	2A	1473	C
1	2A	1490	A
1	2A	1499	A
1	2A	1503	A
1	2A	1505	G
1	2A	1506	A
1	2A	1513	C
1	2A	1515	A
1	2A	1517	A
1	2A	1528	G

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Mol	Chain	Res	Type
1	2A	1538	C
1	2A	1539	A
1	2A	1542	U
1	2A	1553	A
1	2A	1554	C
1	2A	1555	A
1	2A	1556	A
1	2A	1577	C
1	2A	1579	G
1	2A	1588	A
1	2A	1589	C
1	2A	1593	C
1	2A	1604	A
1	2A	1605	G
1	2A	1615	A
1	2A	1624	U
1	2A	1626	A
1	2A	1630	C
1	2A	1631	A
1	2A	1653	A
1	2A	1654	A
1	2A	1655	A
1	2A	1661	A
1	2A	1663	A
1	2A	1676	C
1	2A	1682	C
1	2A	1694	C
1	2A	1710	A
1	2A	1716	C
1	2A	1718	C
1	2A	1720	G
1	2A	1737	C
1	2A	1742	G
1	2A	1746	A
1	2A	1766	A
1	2A	1775	G
1	2A	1786	G
1	2A	1793	G
1	2A	1794	G
1	2A	1803	A
1	2A	1810	A
1	2A	1811	C

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Mol	Chain	Res	Type
1	2A	1821	A
1	2A	1830	C
1	2A	1831	G
1	2A	1832	A
1	2A	1838	U
1	2A	1846	G
1	2A	1856	G
1	2A	1865	G
1	2A	1873	C
1	2A	1877	A
1	2A	1878	A
1	2A	1891	G
1	2A	1898	A
1	2A	1899	G
1	2A	1924	G
1	2A	1927	G
1	2A	1933	A
1	2A	1934	A
1	2A	1935	C
1	2A	1950	G
1	2A	1951	G
1	2A	1963	5MC
1	2A	1976	U
1	2A	1984	U
1	2A	1985	G
1	2A	1988	C
1	2A	1990	A
1	2A	1991	A
1	2A	1992	A
1	2A	1993	A
1	2A	2005	G
1	2A	2013	G
1	2A	2014	U
1	2A	2018	G
1	2A	2041	A
1	2A	2044	G
1	2A	2051	A
1	2A	2052	A
1	2A	2054	A
1	2A	2064	C
1	2A	2070	G
1	2A	2076	C

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Mol	Chain	Res	Type
1	2A	2077	G
1	2A	2081	A
1	2A	2082	G
1	2A	2083	A
1	2A	2087	C
1	2A	2090	G
1	2A	2109	G
1	2A	2114	G
1	2A	2117	U
1	2A	2120	U
1	2A	2124	C
1	2A	2125	G
1	2A	2126	C
1	2A	2128	C
1	2A	2129	C
1	2A	2130	U
1	2A	2131	G
1	2A	2132	C
1	2A	2133	G
1	2A	2137	G
1	2A	2138	A
1	2A	2142	G
1	2A	2147	A
1	2A	2148	G
1	2A	2150	C
1	2A	2152	G
1	2A	2153	U
1	2A	2154	G
1	2A	2155	A
1	2A	2157	C
1	2A	2159	C
1	2A	2166	C
1	2A	2167	C
1	2A	2168	G
1	2A	2169	G
1	2A	2172	G
1	2A	2178	G
1	2A	2179	A
1	2A	2180	G
1	2A	2181	G
1	2A	2182	C
1	2A	2184	C

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Mol	Chain	Res	Type
1	2A	2185	C
1	2A	2186	G
1	2A	2188	U
1	2A	2189	G
1	2A	2193	U
1	2A	2194	A
1	2A	2195	C
1	2A	2198	C
1	2A	2201	U
1	2A	2210	U
1	2A	2213	G
1	2A	2214	G
1	2A	2219	A
1	2A	2226	G
1	2A	2227	G
1	2A	2228	A
1	2A	2236	A
1	2A	2249	G
1	2A	2250	G
1	2A	2260	U
1	2A	2280	A
1	2A	2284	A
1	2A	2286	C
1	2A	2287	G
1	2A	2290	G
1	2A	2294	C
1	2A	2298	A
1	2A	2299	A
1	2A	2316	A
1	2A	2317	C
1	2A	2319	G
1	2A	2322	A
1	2A	2323	U
1	2A	2330	G
1	2A	2331	A
1	2A	2332	G
1	2A	2333	A
1	2A	2336	G
1	2A	2345	G
1	2A	2346	A
1	2A	2347	A
1	2A	2354	C

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Mol	Chain	Res	Type
1	2A	2355	U
1	2A	2358	C
1	2A	2365	G
1	2A	2366	C
1	2A	2376	G
1	2A	2377	A
1	2A	2390	G
1	2A	2394	G
1	2A	2396	C
1	2A	2407	G
1	2A	2417	U
1	2A	2433	A
1	2A	2434	U
1	2A	2436	A
1	2A	2439	G
1	2A	2440	G
1	2A	2441	A
1	2A	2445	A
1	2A	2446	A
1	2A	2450	A
1	2A	2452	C
1	2A	2456	G
1	2A	2459	A
1	2A	2480	A
1	2A	2481	G
1	2A	2485	C
1	2A	2487	A
1	2A	2493	G
1	2A	2513	G
1	2A	2515	U
1	2A	2516	G
1	2A	2517	U
1	2A	2524	G
1	2A	2526	C
1	2A	2529	A
1	2A	2531	C
1	2A	2541	A
1	2A	2560	G
1	2A	2565	U
1	2A	2577	A
1	2A	2578	G
1	2A	2583	A

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Mol	Chain	Res	Type
1	2A	2584	C
1	2A	2587	G
1	2A	2588	A
1	2A	2589	G
1	2A	2611	A
1	2A	2612	C
1	2A	2613	A
1	2A	2614	G
1	2A	2622	U
1	2A	2623	C
1	2A	2626	U
1	2A	2640	A
1	2A	2641	G
1	2A	2657	C
1	2A	2665	A
1	2A	2674	G
1	2A	2690	A
1	2A	2692	C
1	2A	2700	U
1	2A	2701	C
1	2A	2713	U
1	2A	2724	A
1	2A	2725	A
1	2A	2726	G
1	2A	2738	U
1	2A	2745	A
1	2A	2756	G
1	2A	2760	A
1	2A	2762	A
1	2A	2771	G
1	2A	2777	A
1	2A	2787	A
1	2A	2790	A
1	2A	2827	G
1	2A	2829	A
1	2A	2830	A
1	2A	2842	G
1	2A	2848	G
1	2A	2856	U
1	2A	2881	G
1	2A	2889	C
1	2A	2890	C

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Mol	Chain	Res	Type
1	2A	2891	A
1	2A	2900	A
1	2A	2902	G
2	2B	2	C
2	2B	5	C
2	2B	8	U
2	2B	13	A
2	2B	30	C
2	2B	31	C
2	2B	33	G
2	2B	42	C
2	2B	51	G
2	2B	56	G
2	2B	73	A
2	2B	75	G
2	2B	84	C
2	2B	91	C
2	2B	106	G
2	2B	110	G
2	2B	120	A
32	2a	6	U
32	2a	7	G
32	2a	8	G
32	2a	9	A
32	2a	10	G
32	2a	23	G
32	2a	32	G
32	2a	33	A
32	2a	40	G
32	2a	48	C
32	2a	49	C
32	2a	52	A
32	2a	53	G
32	2a	62	G
32	2a	66	U
32	2a	67	G
32	2a	85	C
32	2a	110	A
32	2a	114	A
32	2a	115	C
32	2a	125	A
32	2a	126	C

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Mol	Chain	Res	Type
32	2a	139	G
32	2a	151	G
32	2a	158	C
32	2a	168	U
32	2a	169	C
32	2a	177	U
32	2a	190	U
32	2a	194	G
32	2a	202	A
32	2a	208	C
32	2a	209	U
32	2a	210	U
32	2a	211	U
32	2a	212	G
32	2a	243	G
32	2a	245	U
32	2a	246	A
32	2a	247	G
32	2a	262	G
32	2a	263	C
32	2a	282	G
32	2a	285	G
32	2a	286	C
32	2a	301	G
32	2a	324	C
32	2a	328	G
32	2a	342	G
32	2a	344	G
32	2a	345	A
32	2a	347	G
32	2a	348	C
32	2a	349	A
32	2a	350	G
32	2a	363	U
32	2a	368	C
32	2a	369	A
32	2a	384	G
32	2a	393	A
32	2a	394	C
32	2a	402	G
32	2a	406	G
32	2a	407	A

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Mol	Chain	Res	Type
32	2a	408	A
32	2a	409	G
32	2a	417	U
32	2a	419	G
32	2a	424	G
32	2a	425	U
32	2a	426	A
32	2a	435	A
32	2a	437	C
32	2a	441	G
32	2a	447	A
32	2a	448	A
32	2a	453	C
32	2a	455	A
32	2a	456	C
32	2a	462	G
32	2a	467	A
32	2a	470	G
32	2a	481	A
32	2a	482	U
32	2a	484	G
32	2a	489	G
32	2a	493	A
32	2a	494	A
32	2a	495	C
32	2a	501	G
32	2a	502	C
32	2a	505	G
32	2a	511	G7M
32	2a	512	C
32	2a	516	A
32	2a	517	A
32	2a	518	U
32	2a	531	A
32	2a	543	A
32	2a	545	U
32	2a	546	C
32	2a	548	C
32	2a	556	A
32	2a	557	A
32	2a	559	G
32	2a	560	G

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Mol	Chain	Res	Type
32	2a	561	G
32	2a	600	G
32	2a	614	G
32	2a	617	G
32	2a	636	U
32	2a	637	A
32	2a	649	A
32	2a	650	G
32	2a	671	A
32	2a	672	G
32	2a	679	A
32	2a	705	G
32	2a	707	U
32	2a	714	G
32	2a	716	C
32	2a	718	G
32	2a	733	C
32	2a	735	U
32	2a	737	A
32	2a	743	A
32	2a	758	G
32	2a	761	A
32	2a	774	A
32	2a	777	U
32	2a	778	A
32	2a	801	C
32	2a	812	A
32	2a	823	U
32	2a	824	C
32	2a	825	U
32	2a	828	U
32	2a	831	G
32	2a	837	A
32	2a	851	A
32	2a	852	G
32	2a	856	G
32	2a	868	G
32	2a	880	G
32	2a	892	A
32	2a	894	G
32	2a	904	G
32	2a	905	G

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Mol	Chain	Res	Type
32	2a	912	C
32	2a	913	A
32	2a	916	A
32	2a	939	U
32	2a	943	A
32	2a	946	A
32	2a	947	A
32	2a	949	G
32	2a	950	C
32	2a	952	A
32	2a	953	A
32	2a	954	G
32	2a	955	A
32	2a	967	C
32	2a	970	U
32	2a	971	G
32	2a	972	A
32	2a	978	U
32	2a	983	A
32	2a	984	A
32	2a	985	C
32	2a	988	G
32	2a	995	A
32	2a	998	C
32	2a	999	U
32	2a	1001	G
32	2a	1002	G
32	2a	1004	U
32	2a	1005	G
32	2a	1006	C
32	2a	1007	C
32	2a	1009	C
32	2a	1010	G
32	2a	1011	C
32	2a	1021	C
32	2a	1024	A
32	2a	1026	C
32	2a	1037	C
32	2a	1048	U
32	2a	1049	C
32	2a	1051	G
32	2a	1077	G

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Mol	Chain	Res	Type
32	2a	1078	U
32	2a	1082	G
32	2a	1084	A
32	2a	1100	G
32	2a	1108	U
32	2a	1112	C
32	2a	1113	A
32	2a	1119	U
32	2a	1120	C
32	2a	1121	G
32	2a	1122	G
32	2a	1130	C
32	2a	1135	A
32	2a	1140	A
32	2a	1142	U
32	2a	1165	A
32	2a	1166	G
32	2a	1178	U
32	2a	1179	G
32	2a	1180	G
32	2a	1182	C
32	2a	1195	A
32	2a	1198	G
32	2a	1206	G
32	2a	1209	A
32	2a	1220	A
32	2a	1227	A
32	2a	1232	A
32	2a	1238	A
32	2a	1239	U
32	2a	1240	G
32	2a	1242	C
32	2a	1249	C
32	2a	1252	C
32	2a	1259	C
32	2a	1260	U
32	2a	1261	A
32	2a	1262	A
32	2a	1263	U
32	2a	1264	C
32	2a	1269	A
32	2a	1271	A

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Mol	Chain	Res	Type
32	2a	1275	G
32	2a	1282	G
32	2a	1283	U
32	2a	1284	U
32	2a	1287	G
32	2a	1294	G
32	2a	1298	G
32	2a	1299	C
32	2a	1302	C
32	2a	1317	C
32	2a	1320	G
32	2a	1328	A
32	2a	1329	G
32	2a	1335	G
32	2a	1345	C
32	2a	1346	A
32	2a	1353	G
32	2a	1361	C
32	2a	1362	G
32	2a	1383	5MC
32	2a	1384	G
32	2a	1401	A
32	2a	1402	G
32	2a	1412	C
32	2a	1425	G
32	2a	1426	G
32	2a	1432	A
32	2a	1433	C
32	2a	1465	G
32	2a	1470	A
32	2a	1475	G
32	2a	1481	A
32	2a	1482	G
32	2a	1484	U
32	2a	1485	A
32	2a	1495	G
32	2a	1498	G
32	2a	1507	G
32	2a	1508	G

All (60) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	301	A
1	1A	516	A
1	1A	715	G
1	1A	933	A
1	1A	934	C
1	1A	940	U
1	1A	1218	A
1	1A	1219	U
1	1A	1220	G
1	1A	1254	A
1	1A	1320	A
1	1A	1345	U
1	1A	1425	G
1	1A	1625	A
1	1A	1699	G
1	1A	1709	C
1	1A	2132	C
1	1A	2147	A
1	1A	2218	U
1	1A	2613	A
1	1A	2700	U
1	1A	2768	U
1	2A	8	U
1	2A	183	A
1	2A	202	G
1	2A	272	G
1	2A	300	C
1	2A	357	C
1	2A	367	G
1	2A	668	A
1	2A	742	G
1	2A	798	A
1	2A	846	A
1	2A	902	C
1	2A	945	A
1	2A	1039	C
1	2A	1098	C
1	2A	1102	A
1	2A	1110	U
1	2A	1112	A
1	2A	1118	A
1	2A	1121	C
1	2A	1254	A

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Mol	Chain	Res	Type
1	2A	1294	U
1	2A	1320	A
1	2A	1424	A
1	2A	1425	G
1	2A	1465	U
1	2A	1469	G
1	2A	1555	A
1	2A	1709	C
1	2A	1820	C
1	2A	2013	G
1	2A	2147	A
1	2A	2192	A
1	2A	2193	U
1	2A	2332	G
1	2A	2613	A
1	2A	2673	A
1	2A	2700	U

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

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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

All (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
43	1l	92	0TD	CB-SB	-5.94	1.69	1.84
32	1a	511	G7M	C5-C4	5.87	1.47	1.39
43	2l	92	0TD	CB-SB	-5.82	1.70	1.84
1	1A	2514	2MA	C6-C5	4.83	1.48	1.41
32	1a	1387	5MC	C5-C4	4.80	1.48	1.41
32	2a	1390	5MC	C5-C4	4.80	1.48	1.41
1	2A	1983	5MC	C5-C4	4.79	1.48	1.41
1	1A	1983	5MC	C5-C4	4.77	1.48	1.41
32	1a	1383	5MC	C5-C4	4.77	1.48	1.41
1	2A	2514	2MA	C6-C5	4.77	1.48	1.41
32	2a	1383	5MC	C5-C4	4.77	1.48	1.41
32	1a	945	5MC	C5-C4	4.76	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1963	5MC	C5-C4	4.74	1.48	1.41
32	1a	1390	5MC	C5-C4	4.74	1.48	1.41
1	2A	1932	PSU	C5-C1'	-4.73	1.48	1.52
1	2A	2616	PSU	C5-C1'	-4.73	1.48	1.52
32	2a	945	5MC	C5-C4	4.72	1.48	1.41
1	2A	1963	5MC	C5-C4	4.71	1.48	1.41
1	2A	1938	PSU	C5-C1'	-4.63	1.48	1.52
32	2a	1387	5MC	C5-C4	4.61	1.48	1.41
32	2a	500	PSU	C5-C1'	-4.51	1.48	1.52
1	1A	1938	PSU	C5-C1'	-4.44	1.48	1.52
1	1A	2616	PSU	C5-C1'	-4.39	1.48	1.52
32	1a	1189	2MG	C6-C5	4.31	1.48	1.41
32	2a	1189	2MG	C6-C5	4.20	1.48	1.41
32	1a	944	M2G	C6-C5	4.18	1.48	1.41
32	2a	944	M2G	C6-C5	4.16	1.48	1.41
1	1A	1932	PSU	C5-C1'	-4.16	1.48	1.52
1	1A	2262	OMG	C6-C5	4.12	1.48	1.41
32	1a	500	PSU	C5-C1'	-4.08	1.48	1.52
1	2A	2262	OMG	C6-C5	4.07	1.48	1.41
32	1a	511	G7M	C6-C5	3.91	1.48	1.41
32	2a	511	G7M	C6-C5	3.83	1.48	1.41
1	1A	1960	5MU	C4-C5	3.46	1.48	1.41
1	2A	1960	5MU	C4-C5	3.41	1.48	1.41
32	2a	944	M2G	C2-N2	3.39	1.40	1.34
1	2A	1938	PSU	C4-C5	3.36	1.48	1.41
1	2A	1936	5MU	C4-C5	3.36	1.48	1.41
32	2a	500	PSU	C4-C5	3.36	1.48	1.41
1	1A	1932	PSU	C4-C5	3.35	1.48	1.41
32	1a	944	M2G	C2-N2	3.33	1.40	1.34
1	1A	1938	PSU	C4-C5	3.33	1.48	1.41
1	2A	1932	PSU	C4-C5	3.32	1.48	1.41
1	2A	2616	PSU	C4-C5	3.32	1.48	1.41
1	1A	2616	PSU	C4-C5	3.32	1.48	1.41
1	1A	1936	5MU	C4-C5	3.31	1.48	1.41
32	1a	500	PSU	C4-C5	3.28	1.48	1.41
32	2a	1496	MA6	C5-C4	2.56	1.47	1.40
32	2a	944	M2G	C5-C4	2.52	1.47	1.40
32	1a	1497	MA6	C5-C4	2.51	1.47	1.40
32	1a	944	M2G	C5-C4	2.50	1.47	1.40
32	1a	1496	MA6	C5-C4	2.50	1.47	1.40
32	2a	1189	2MG	C5-C4	2.49	1.47	1.40
32	2a	1497	MA6	C5-C4	2.46	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2262	OMG	C5-C4	2.45	1.47	1.40
1	2A	2514	2MA	C5-C4	2.44	1.47	1.40
1	1A	2514	2MA	C5-C4	2.43	1.47	1.40
32	1a	1189	2MG	C5-C4	2.42	1.47	1.40
1	2A	2262	OMG	C5-C4	2.40	1.47	1.40
32	1a	500	PSU	O4'-C1'	-2.12	1.41	1.44
32	2a	500	PSU	O4'-C1'	-2.10	1.41	1.44
1	1A	1938	PSU	O4'-C1'	-2.08	1.41	1.44
1	1A	1960	5MU	C2-N3	-2.01	1.34	1.38

All (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
1	1A	1938	PSU	N1-C2-N3	-8.21	121.91	128.43
1	2A	1938	PSU	N1-C2-N3	-8.19	121.92	128.43
1	1A	2616	PSU	N1-C2-N3	-8.18	121.93	128.43
1	2A	2616	PSU	N1-C2-N3	-8.18	121.93	128.43
1	2A	1932	PSU	N1-C2-N3	-8.12	121.98	128.43
1	2A	1936	5MU	C4-N3-C2	6.82	120.90	115.14
1	1A	1936	5MU	C4-N3-C2	6.79	120.87	115.14
1	1A	2514	2MA	C2-N3-C4	6.67	120.94	115.52
1	2A	1938	PSU	C4-N3-C2	6.66	120.77	115.14
1	1A	1938	PSU	C4-N3-C2	6.65	120.76	115.14
1	2A	2514	2MA	C2-N3-C4	6.61	120.89	115.52
1	2A	1932	PSU	C4-N3-C2	6.58	120.70	115.14
1	1A	1932	PSU	C4-N3-C2	6.52	120.65	115.14
1	2A	2616	PSU	C4-N3-C2	6.47	120.61	115.14
1	1A	2616	PSU	C4-N3-C2	6.47	120.60	115.14
32	2a	500	PSU	C4-N3-C2	6.44	120.58	115.14
1	2A	1960	5MU	C4-N3-C2	6.35	120.50	115.14
32	1a	500	PSU	C4-N3-C2	6.29	120.46	115.14
1	1A	1960	5MU	C4-N3-C2	6.25	120.42	115.14
32	2a	511	G7M	C5-C6-N1	-5.72	115.61	123.43
32	1a	511	G7M	C5-C6-N1	-5.65	115.71	123.43
1	2A	1938	PSU	C5-C4-N3	-5.53	118.23	125.36
1	2A	1932	PSU	C5-C4-N3	-5.49	118.29	125.36
1	1A	1938	PSU	C5-C4-N3	-5.44	118.36	125.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2616	PSU	C5-C4-N3	-5.40	118.41	125.36
1	1A	1932	PSU	C5-C4-N3	-5.34	118.48	125.36
1	1A	2616	PSU	C5-C4-N3	-5.34	118.49	125.36
32	2a	500	PSU	C5-C4-N3	-5.27	118.56	125.36
32	1a	944	M2G	C6-N1-C2	5.17	122.34	116.18
32	1a	500	PSU	C5-C4-N3	-5.15	118.72	125.36
32	2a	944	M2G	C6-N1-C2	5.13	122.29	116.18
1	2A	2616	PSU	C5-C1'-C2'	-5.10	106.23	115.32
32	1a	1189	2MG	C2-N3-C4	5.06	121.03	115.28
32	2a	944	M2G	C2-N3-C4	4.95	120.90	115.28
32	1a	944	M2G	C2-N3-C4	4.95	120.90	115.28
32	2a	1189	2MG	C2-N3-C4	4.95	120.90	115.28
1	2A	2262	OMG	C2-N3-C4	4.91	120.97	115.36
1	1A	2262	OMG	C2-N3-C4	4.88	120.92	115.36
1	2A	2514	2MA	C5-C6-N1	-4.87	117.95	123.06
1	1A	2514	2MA	C5-C6-N1	-4.86	117.96	123.06
32	2a	500	PSU	C5-C6-N1	-4.64	118.74	124.44
32	1a	500	PSU	C5-C6-N1	-4.60	118.79	124.44
32	1a	1497	MA6	N1-C6-N6	4.56	121.85	117.06
1	1A	2262	OMG	C6-N1-C2	4.47	123.04	115.93
32	2a	500	PSU	C6-N1-C2	4.47	122.73	115.36
1	2A	2616	PSU	C5-C6-N1	-4.38	119.06	124.44
1	1A	2616	PSU	C5-C6-N1	-4.38	119.06	124.44
32	1a	500	PSU	C6-N1-C2	4.36	122.55	115.36
1	1A	1932	PSU	C5-C6-N1	-4.33	119.11	124.44
1	2A	1938	PSU	C5-C1'-C2'	-4.33	107.59	115.32
32	2a	511	G7M	C6-N1-C2	4.32	122.79	115.93
32	1a	511	G7M	C6-N1-C2	4.31	122.78	115.93
32	2a	1497	MA6	N1-C6-N6	4.29	121.57	117.06
1	2A	1932	PSU	C5-C6-N1	-4.27	119.19	124.44
1	2A	1938	PSU	C5-C6-N1	-4.20	119.27	124.44
1	1A	2262	OMG	C5-C6-N1	-4.19	117.70	123.43
1	1A	1941	OMC	C2-N3-C4	4.17	120.57	116.34
1	1A	1932	PSU	C6-N1-C2	4.13	122.18	115.36
1	1A	1938	PSU	C5-C6-N1	-4.13	119.36	124.44
32	2a	1189	2MG	C6-N1-C2	4.13	122.58	115.18
1	1A	2616	PSU	C6-N1-C2	4.12	122.16	115.36
32	2a	1189	2MG	C5-C6-N1	-4.11	117.81	123.43
1	2A	2616	PSU	C6-N1-C2	4.11	122.14	115.36
1	2A	2262	OMG	C6-C5-C4	-4.07	116.91	120.80
32	1a	944	M2G	C5-C6-N1	-4.06	117.88	123.43
32	2a	944	M2G	C5-C6-N1	-4.04	117.91	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1938	PSU	C6-N1-C2	4.02	122.00	115.36
1	2A	1932	PSU	C6-N1-C2	4.02	121.99	115.36
32	1a	511	G7M	C2-N3-C4	4.01	119.93	115.36
1	1A	2262	OMG	C6-C5-C4	-4.00	116.98	120.80
1	1A	1938	PSU	C6-N1-C2	4.00	121.96	115.36
1	2A	2262	OMG	C6-N1-C2	3.99	122.27	115.93
1	2A	1932	PSU	C5-C1'-C2'	-3.99	108.20	115.32
32	2a	511	G7M	C2-N3-C4	3.98	119.90	115.36
32	1a	1189	2MG	C5-C6-N1	-3.93	118.06	123.43
32	1a	1189	2MG	C6-N1-C2	3.87	122.11	115.18
32	1a	1496	MA6	N1-C6-N6	3.85	121.11	117.06
1	2A	1941	OMC	C2-N3-C4	3.85	120.24	116.34
32	1a	1189	2MG	C6-C5-C4	-3.82	117.15	120.80
1	1A	2616	PSU	C5-C1'-C2'	-3.68	108.76	115.32
1	2A	2262	OMG	C5-C6-N1	-3.66	118.42	123.43
1	1A	2262	OMG	N3-C2-N1	-3.63	122.38	127.22
32	1a	1390	5MC	C2-N3-C4	3.63	120.40	116.02
32	2a	1189	2MG	C6-C5-C4	-3.62	117.34	120.80
32	2a	945	5MC	C2-N3-C4	3.59	120.36	116.02
32	1a	1383	5MC	C2-N3-C4	3.59	120.35	116.02
32	1a	945	5MC	C2-N3-C4	3.56	120.31	116.02
32	1a	944	M2G	C6-C5-C4	-3.55	117.41	120.80
32	2a	1387	5MC	C2-N3-C4	3.54	120.29	116.02
32	2a	944	M2G	C6-C5-C4	-3.54	117.42	120.80
1	2A	1963	5MC	C2-N3-C4	3.54	120.28	116.02
32	2a	1383	5MC	C2-N3-C4	3.52	120.27	116.02
32	1a	1387	5MC	C2-N3-C4	3.51	120.25	116.02
32	2a	1390	5MC	C2-N3-C4	3.49	120.23	116.02
32	1a	1385	4OC	CM4-N4-C4	-3.49	119.97	122.97
32	2a	1497	MA6	C9-N6-C6	-3.48	108.96	119.51
1	1A	1963	5MC	C2-N3-C4	3.47	120.20	116.02
32	2a	1385	4OC	CM4-N4-C4	-3.45	120.01	122.97
1	1A	1983	5MC	C2-N3-C4	3.43	120.16	116.02
1	2A	1983	5MC	C2-N3-C4	3.42	120.15	116.02
32	2a	1497	MA6	C10-N6-C6	-3.41	109.18	119.51
32	2a	1496	MA6	C9-N6-C6	-3.41	109.20	119.51
1	2A	2262	OMG	N3-C2-N1	-3.40	122.69	127.22
32	1a	1496	MA6	C9-N6-C6	-3.29	109.54	119.51
32	1a	1496	MA6	C10-N6-C6	-3.23	109.73	119.51
32	2a	1496	MA6	N3-C2-N1	-3.22	123.65	128.68
32	1a	1496	MA6	N3-C2-N1	-3.19	123.70	128.68
32	1a	1497	MA6	C10-N6-C6	-3.18	109.87	119.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1497	MA6	C9-N6-C6	-3.17	109.92	119.51
32	2a	1497	MA6	N3-C2-N1	-3.13	123.79	128.68
32	1a	1497	MA6	N3-C2-N1	-3.07	123.87	128.68
32	2a	1496	MA6	C4-C5-N7	-3.00	106.27	109.40
32	1a	1189	2MG	C4-C5-N7	-2.97	106.31	109.40
32	2a	1387	5MC	N4-C4-N3	2.97	121.23	117.03
1	1A	1960	5MU	C5-C6-N1	-2.96	119.00	122.19
32	1a	1189	2MG	CM2-N2-C2	-2.95	120.03	123.59
32	2a	1496	MA6	N1-C6-N6	2.90	120.11	117.06
32	2a	1189	2MG	CM2-N2-C2	-2.85	120.15	123.59
1	1A	2514	2MA	C4-C5-N7	-2.84	106.44	109.40
1	2A	1960	5MU	C5-C6-N1	-2.80	119.18	122.19
32	2a	1496	MA6	C10-N6-C6	-2.75	111.19	119.51
1	2A	2514	2MA	C4-C5-N7	-2.69	106.59	109.40
32	1a	1496	MA6	C4-C5-N7	-2.67	106.62	109.40
32	2a	511	G7M	CN7-N7-C8	-2.60	112.91	125.43
32	1a	511	G7M	CN7-N7-C8	-2.58	113.04	125.43
32	2a	1189	2MG	C4-C5-N7	-2.55	106.74	109.40
32	1a	944	M2G	C4-C5-N7	-2.55	106.74	109.40
1	1A	1983	5MC	C5-C6-N1	-2.54	119.46	122.19
1	2A	1983	5MC	C5-C6-N1	-2.53	119.47	122.19
32	1a	511	G7M	N3-C2-N1	-2.51	123.88	127.22
1	1A	2262	OMG	C4-C5-N7	-2.51	106.79	109.40
32	1a	1390	5MC	N4-C4-N3	2.50	120.57	117.03
32	2a	1497	MA6	C4-C5-N7	-2.49	106.80	109.40
1	2A	1983	5MC	N4-C4-N3	2.49	120.55	117.03
32	1a	1383	5MC	N4-C4-N3	2.49	120.55	117.03
1	1A	1963	5MC	C5-C6-N1	-2.49	119.52	122.19
1	2A	1941	OMC	N4-C4-N3	2.46	120.38	116.49
32	2a	1390	5MC	N4-C4-N3	2.46	120.51	117.03
32	2a	1383	5MC	C5-C6-N1	-2.45	119.56	122.19
32	1a	945	5MC	N4-C4-N3	2.45	120.49	117.03
32	2a	944	M2G	C4-C5-N7	-2.45	106.85	109.40
32	2a	1497	MA6	C10-N6-C9	-2.45	108.24	116.12
32	1a	1387	5MC	C5-C6-N1	-2.44	119.56	122.19
32	2a	511	G7M	N3-C2-N1	-2.44	123.97	127.22
32	2a	511	G7M	C1'-N9-C4	2.43	130.91	126.64
32	2a	1390	5MC	C5-C6-N1	-2.42	119.58	122.19
1	1A	1963	5MC	N4-C4-N3	2.42	120.45	117.03
32	1a	1387	5MC	N4-C4-N3	2.42	120.45	117.03
32	2a	945	5MC	N4-C4-N3	2.41	120.44	117.03
1	2A	1963	5MC	N4-C4-N3	2.40	120.43	117.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1383	5MC	N4-C4-N3	2.39	120.41	117.03
1	1A	1983	5MC	N4-C4-N3	2.39	120.41	117.03
1	2A	2262	OMG	C4-C5-N7	-2.39	106.91	109.40
1	2A	1963	5MC	C5-C6-N1	-2.37	119.64	122.19
32	1a	1497	MA6	C4-C5-N7	-2.36	106.94	109.40
32	2a	945	5MC	C5-C6-N1	-2.34	119.68	122.19
32	1a	945	5MC	C5-C6-N1	-2.30	119.71	122.19
32	2a	1387	5MC	C5-C6-N1	-2.28	119.74	122.19
32	1a	1383	5MC	C5-C6-N1	-2.27	119.75	122.19
1	1A	1941	OMC	N4-C4-N3	2.24	120.03	116.49
32	1a	1390	5MC	C5-C6-N1	-2.18	119.85	122.19
1	2A	1936	5MU	C5-C6-N1	-2.16	119.87	122.19
32	2a	1189	2MG	N3-C2-N1	-2.16	122.82	126.23
32	1a	500	PSU	O4'-C1'-C2'	2.15	108.14	104.66
32	2a	500	PSU	O4'-C1'-C2'	2.15	108.14	104.66
1	1A	1936	5MU	C5-C6-N1	-2.13	119.90	122.19
1	1A	1932	PSU	C5-C1'-C2'	-2.12	111.53	115.32
1	1A	1938	PSU	C5-C1'-C2'	-2.11	111.56	115.32
32	1a	1189	2MG	N3-C2-N1	-2.06	122.97	126.23
32	2a	1496	MA6	C10-N6-C9	-2.06	109.50	116.12
32	2a	500	PSU	C5-C1'-C2'	-2.04	111.67	115.32
1	1A	1932	PSU	O4'-C1'-C2'	2.02	107.93	104.66
32	1a	1496	MA6	C10-N6-C9	-2.01	109.63	116.12

There are no chirality outliers.

All (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
32	1a	1497	MA6	O4'-C4'-C5'-O5'
1	1A	1960	5MU	C2'-C1'-N1-C6
1	1A	1960	5MU	O4'-C1'-N1-C6
32	1a	1383	5MC	O4'-C4'-C5'-O5'
32	1a	1383	5MC	C3'-C4'-C5'-O5'
1	1A	1941	OMC	C2'-C1'-N1-C6
32	2a	1383	5MC	O4'-C4'-C5'-O5'
32	2a	1385	4OC	N3-C4-N4-CM4
32	2a	1385	4OC	C5-C4-N4-CM4

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Mol	Chain	Res	Type	Atoms
32	2a	1497	MA6	O4'-C4'-C5'-O5'
32	2a	1497	MA6	C5-C6-N6-C9
32	2a	511	G7M	C3'-C4'-C5'-O5'
1	2A	1941	OMC	C2'-C1'-N1-C6
32	1a	1476	UR3	O4'-C1'-N1-C6
32	1a	1476	UR3	C2'-C1'-N1-C6
32	2a	1496	MA6	C5-C6-N6-C9
32	2a	1496	MA6	C5-C6-N6-C10
32	2a	944	M2G	N1-C2-N2-CM1
32	2a	944	M2G	N3-C2-N2-CM2
1	2A	2514	2MA	O4'-C4'-C5'-O5'
32	1a	1497	MA6	C3'-C4'-C5'-O5'
32	2a	1383	5MC	C3'-C4'-C5'-O5'
32	2a	1385	4OC	O4'-C4'-C5'-O5'
32	2a	1497	MA6	C3'-C4'-C5'-O5'
1	2A	1963	5MC	C3'-C4'-C5'-O5'
32	2a	1385	4OC	C3'-C4'-C5'-O5'
32	2a	1497	MA6	N1-C6-N6-C9
32	2a	944	M2G	N1-C2-N2-CM2
32	2a	944	M2G	N3-C2-N2-CM1
32	2a	1496	MA6	N1-C6-N6-C9
32	2a	511	G7M	O4'-C4'-C5'-O5'
32	2a	1497	MA6	C5-C6-N6-C10
1	2A	1941	OMC	C3'-C2'-O2'-CM2
1	2A	2514	2MA	C3'-C4'-C5'-O5'
32	1a	1497	MA6	C5-C6-N6-C10
32	1a	1496	MA6	C5-C6-N6-C10
32	2a	1497	MA6	C4'-C5'-O5'-P
32	1a	511	G7M	C4'-C5'-O5'-P
32	2a	500	PSU	O4'-C1'-C5-C6
32	2a	500	PSU	O4'-C1'-C5-C4
43	2l	92	0TD	CA-CB-SB-CSB
1	1A	2514	2MA	O4'-C4'-C5'-O5'
1	1A	1938	PSU	C2'-C1'-C5-C6
1	2A	1938	PSU	C2'-C1'-C5-C6
1	1A	2563	OMU	O4'-C4'-C5'-O5'
43	1l	92	0TD	CG-CB-SB-CSB
32	1a	511	G7M	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	-

All (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
56	1A	3801	FSD	CAQ-CBF	2.76	1.46	1.39
56	2A	3553	FSD	CAR-CAQ	-2.75	1.32	1.38
56	2A	3553	FSD	CAC-NBP	2.62	1.55	1.46
56	1A	3801	FSD	CBF-NAV	-2.57	1.29	1.34
56	1A	3801	FSD	CAC-NBP	2.54	1.55	1.46
56	1A	3801	FSD	CAD-NBP	2.37	1.54	1.46

All (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
56	2A	3553	FSD	CBI-CBO-NBP	-3.57	101.11	112.38
56	2A	3553	FSD	CBH-OAY-CBM	3.43	119.98	113.47
56	2A	3553	FSD	OAL-CBK-CBJ	-2.86	103.75	110.35
56	2A	3553	FSD	CBN-OAZ-CBI	-2.74	108.95	113.67
56	2A	3553	FSD	OBA-CBL-CAT	2.64	116.46	109.54
56	1A	3801	FSD	CAQ-CBF-NAV	-2.53	118.90	123.16
56	2A	3553	FSD	CAN-CBD-NAW	-2.47	112.09	120.40
56	1A	3801	FSD	NAX-CBF-NAV	2.43	119.01	113.24
56	2A	3553	FSD	CBN-OBA-CBL	2.38	119.01	115.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	2A	3553	FSD	CAM-CBD-NAW	2.35	128.32	120.40
56	1A	3801	FSD	CBD-NAW-CBC	2.31	130.97	126.78
56	2A	3553	FSD	CAQ-CBF-NAV	-2.27	119.33	123.16
56	2A	3553	FSD	CAD-NBP-CAC	-2.27	103.67	110.38
56	1A	3801	FSD	CAN-CBD-NAW	-2.03	113.56	120.40
56	2A	3553	FSD	OAK-CBJ-CBK	2.01	115.00	110.35

There are no chirality outliers.

All (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
56	2A	3553	FSD	CBK-CBO-NBP-CAD
55	1A	3800	MPD	O2-C2-C3-C4
55	1A	3800	MPD	CM-C2-C3-C4
55	1T	8004	MPD	C1-C2-C3-C4
55	1T	8004	MPD	O2-C2-C3-C4
56	2A	3553	FSD	OAZ-CBN-OBA-CBL
56	2A	3553	FSD	CAN-CBD-NAW-CBC
56	2A	3553	FSD	CAM-CBD-NAW-CBC
56	1A	3801	FSD	OAH-CBC-CBR-CAE
56	2A	3553	FSD	OAH-CBC-CBR-CAE
56	1A	3801	FSD	NAW-CBC-CBR-CAE
56	2A	3553	FSD	NAW-CBC-CBR-CAE
55	2A	3551	MPD	O2-C2-C3-C4
56	2A	3553	FSD	OAJ-CAS-CBR-NAF
56	2A	3553	FSD	OAJ-CAS-CBR-CBC
56	1A	3801	FSD	OAZ-CBN-OBA-CBL
55	2A	3552	MPD	CM-C2-C3-C4
55	1a	1900	MPD	C1-C2-C3-C4
55	2A	3551	MPD	C1-C2-C3-C4
55	2A	3551	MPD	CM-C2-C3-C4
55	1T	8004	MPD	CM-C2-C3-C4
55	18	104	MPD	CM-C2-C3-C4
56	1A	3801	FSD	CBJ-CBN-OBA-CBL
55	2A	3552	MPD	O2-C2-C3-C4
55	18	104	MPD	O2-C2-C3-C4
55	2B	210	MPD	C2-C3-C4-C5

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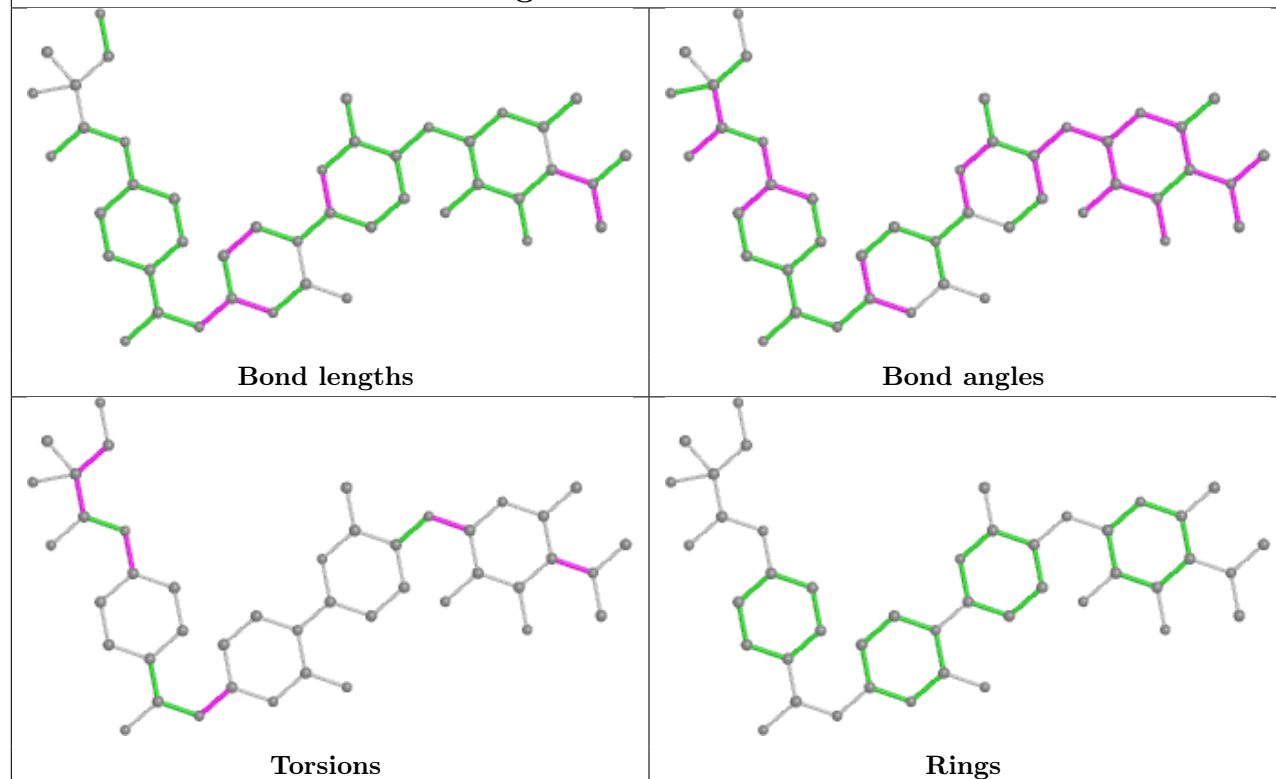
Mol	Chain	Res	Type	Atoms
55	2A	3552	MPD	C2-C3-C4-C5
55	2A	3551	MPD	C2-C3-C4-C5
55	1T	8004	MPD	C2-C3-C4-C5
56	2A	3553	FSD	CBI-CBO-NBP-CAD
55	2B	210	MPD	C2-C3-C4-O4
55	2A	3552	MPD	C2-C3-C4-O4
55	1T	8004	MPD	C2-C3-C4-O4
56	2A	3553	FSD	NAW-CBC-CBR-CAS

There are no ring outliers.

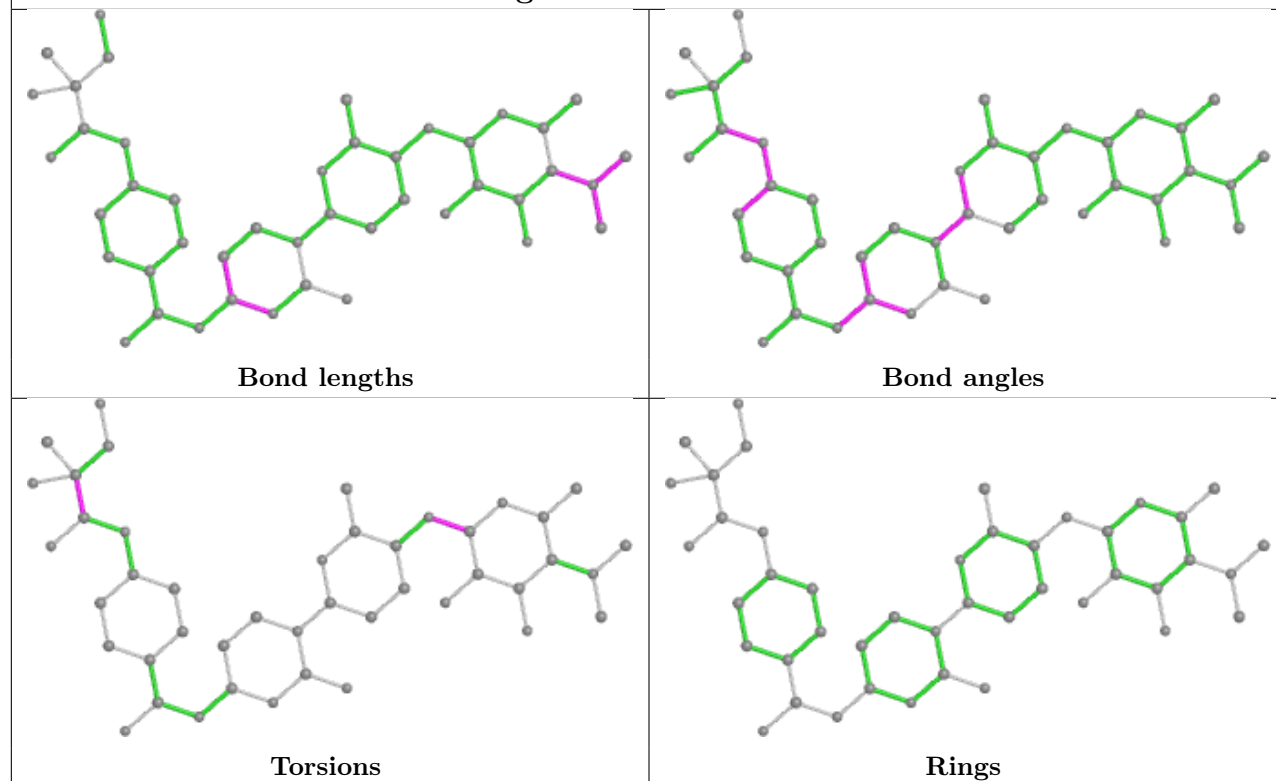
No monomer is involved in short contacts.

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.

Ligand FSD 2A 3553



Ligand FSD 1A 3801



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1A	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 ²)	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 ²)	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 ²)	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

All (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
41	1j	38	ILE	12.8
6	2G	43	LEU	12.7
1	2A	2126	C	12.6
32	2a	1018	A	12.3
1	1A	2140	A	12.0
50	1s	83	HIS	11.7
1	2A	2140	A	11.7
20	2Y	57	GLN	11.6

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Mol	Chain	Res	Type	RSRZ
1	1A	1115	A	11.3
52	2u	5	ASP	11.3
1	2A	2147	A	11.3
40	2i	125	TYR	11.1
1	2A	2193	U	11.1
1	2A	2183	G	11.0
1	1A	2193	U	10.6
44	2m	116	THR	10.4
50	1s	82	GLY	10.3
1	2A	2146	G	10.2
40	2i	126	SER	10.1
1	1A	1119	G	10.1
1	1A	1101	G	10.0
32	2a	1020	C	10.0
1	2A	2152	G	9.9
32	1a	1242	C	9.9
26	24	69	LYS	9.8
50	1s	84	GLY	9.6
44	2m	106	ASN	9.6
6	2G	2	PRO	9.5
32	1a	1018	A	9.5
1	2A	2158	C	9.4
34	1c	39	ILE	9.4
32	1a	923	G	9.4
32	1a	981	G	9.4
48	2q	69	LYS	9.4
52	1u	2	GLY	9.4
1	2A	2192	A	9.3
34	1c	65	ALA	9.3
34	2c	57	ILE	9.2
1	1A	1112	A	9.2
38	1g	74	GLU	9.2
1	2A	2139	U	9.2
1	2A	2128	C	9.1
50	2s	69	HIS	9.1
48	2q	66	SER	9.1
1	1A	1140	A	9.0
6	2G	132	ASN	9.0
44	2m	107	ALA	8.9
40	1i	30	GLY	8.9
41	1j	72	VAL	8.9
32	2a	1005	G	8.8

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Mol	Chain	Res	Type	RSRZ
32	2a	982	G	8.8
1	1A	1148	A	8.8
1	1A	1113	G	8.7
1	2A	2174	G	8.7
32	1a	924	A	8.7
38	2g	2	ALA	8.7
1	2A	2188	U	8.7
35	1d	42	GLN	8.7
40	1i	88	TYR	8.6
34	1c	56	ASP	8.6
1	1A	2194	A	8.6
52	2u	8	THR	8.5
1	2A	2129	C	8.5
1	2A	2138	A	8.4
1	1A	2188	U	8.4
1	2A	2131	G	8.4
1	2A	2175	G	8.4
1	1A	1102	A	8.3
1	2A	2185	C	8.3
1	2A	2173	G	8.3
1	2A	2189	G	8.3
32	1a	982	G	8.3
32	2a	1277	G	8.3
6	2G	44	GLY	8.3
32	1a	1005	G	8.2
26	24	62	ARG	8.2
32	2a	986	C	8.1
32	2a	1242	C	8.1
41	1j	36	GLY	8.1
38	1g	156	TRP	8.1
1	2A	2190	A	8.1
1	1A	1134	G	8.1
1	2A	2133	G	8.1
32	1a	916	A	8.1
32	1a	1021	C	8.1
45	1n	2	ALA	8.0
45	2n	2	ALA	8.0
1	1A	2158	C	8.0
32	1a	1017	G	8.0
41	1j	35	SER	8.0
32	2a	971	G	8.0
32	2a	1016	G	8.0

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Mol	Chain	Res	Type	RSRZ
6	2G	157	ILE	7.9
1	2A	2130	U	7.9
32	1a	1020	C	7.9
6	2G	40	ASN	7.9
1	2A	2154	G	7.9
38	1g	37	ASN	7.9
32	2a	1132	C	7.8
1	2A	2187	G	7.8
6	2G	90	LEU	7.8
1	2A	2127	G	7.7
32	2a	1017	G	7.7
38	1g	91	VAL	7.7
34	1c	200	ALA	7.7
32	2a	1015	G	7.7
32	1a	1225	C	7.7
32	2a	1014	G	7.7
41	2j	39	PRO	7.6
32	1a	985	C	7.6
32	2a	1157	G	7.6
32	2a	1011	C	7.6
50	1s	12	ASP	7.6
1	1A	2192	A	7.6
44	1m	12	ASN	7.5
44	1m	65	LYS	7.5
52	2u	24	ARG	7.5
1	2A	2177	G	7.5
1	1A	2153	U	7.5
1	2A	1128	U	7.5
50	1s	29	ARG	7.4
44	2m	5	ALA	7.4
32	2a	1258	G	7.4
32	2a	1006	C	7.3
32	2a	1107	G	7.3
1	1A	1103	G	7.3
1	1A	1149	C	7.3
1	1A	1118	A	7.3
50	1s	49	ILE	7.2
34	1c	207	VAL	7.2
50	1s	11	VAL	7.2
1	1A	1125	C	7.2
32	1a	1198	G	7.2
32	1a	1204	G	7.1

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Mol	Chain	Res	Type	RSRZ
44	1m	60	VAL	7.1
1	1A	1106	U	7.1
50	1s	38	SER	7.1
1	2A	2141	G	7.1
32	2a	1182	C	7.0
50	2s	33	THR	7.0
32	2a	1268	A	7.0
52	1u	5	ASP	7.0
32	2a	970	U	7.0
33	2b	233	SER	7.0
38	2g	92	SER	7.0
32	2a	1211	A	7.0
6	2G	42	GLY	7.0
1	1A	1120	C	7.0
1	2A	2184	C	7.0
32	1a	984	A	7.0
50	2s	52	TYR	7.0
34	2c	77	ILE	7.0
1	1A	1147	C	6.9
32	1a	1253	G	6.9
32	1a	1316	G	6.9
1	2A	2186	G	6.9
14	2S	52	SER	6.8
32	1a	1009	C	6.8
1	2A	1115	A	6.8
32	1a	1195	A	6.8
1	2A	2805	G	6.8
41	2j	40	LEU	6.8
1	1A	1124	C	6.7
26	24	44	THR	6.7
48	1q	65	ILE	6.7
1	2A	2159	C	6.7
32	2a	1278	C	6.7
32	2a	1209	A	6.6
32	1a	971	G	6.6
50	2s	12	ASP	6.6
34	1c	100	ALA	6.6
32	1a	1114	G	6.6
20	2Y	58	GLY	6.6
26	24	63	TYR	6.6
32	2a	997	C	6.6
44	1m	62	ASN	6.6

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Mol	Chain	Res	Type	RSRZ
1	1A	2138	A	6.6
32	2a	1133	U	6.6
26	24	45	GLY	6.6
1	1A	1117	C	6.5
1	2A	2812	G	6.5
26	24	29	PRO	6.5
1	1A	931	C	6.5
1	1A	2189	G	6.5
34	2c	198	VAL	6.5
40	2i	92	TYR	6.4
32	1a	1132	C	6.4
1	1A	1132	G	6.4
41	2j	35	SER	6.4
44	2m	108	ARG	6.4
32	2a	984	A	6.4
32	2a	983	A	6.4
1	2A	2176	G	6.4
1	1A	1133	A	6.4
40	2i	127	LYS	6.4
44	1m	21	TYR	6.3
1	1A	1126	U	6.3
1	1A	2134	U	6.3
32	1a	1014	G	6.3
32	1a	1248	G	6.3
34	1c	189	ALA	6.3
32	1a	1247	G	6.3
34	2c	32	LEU	6.3
6	2G	156	ASP	6.3
6	2G	155	MET	6.3
26	24	19	GLY	6.3
41	2j	29	ARG	6.3
38	2g	90	GLU	6.2
1	2A	2149	C	6.2
50	1s	40	ILE	6.2
1	2A	929	G	6.2
34	2c	197	GLY	6.2
34	1c	60	ALA	6.2
34	2c	64	VAL	6.2
32	2a	1003	G	6.2
32	1a	979	A	6.2
32	1a	1315	A	6.2
32	1a	925	G	6.2

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Mol	Chain	Res	Type	RSRZ
32	1a	1003	G	6.2
32	1a	1254	G	6.2
6	1G	43	LEU	6.2
6	2G	88	ILE	6.2
32	2a	1026	C	6.2
38	1g	99	LEU	6.1
1	2A	2194	A	6.1
32	2a	1146	C	6.1
32	2a	1147	G	6.1
32	1a	1022	C	6.1
40	1i	105	ASP	6.1
40	2i	124	GLN	6.1
32	2a	83	U	6.0
38	1g	153	HIS	6.0
38	2g	83	ALA	6.0
52	2u	7	ARG	6.0
8	1I	79	ILE	6.0
41	1j	10	GLY	6.0
34	1c	64	VAL	6.0
1	2A	2169	G	6.0
50	1s	37	ARG	6.0
1	2A	2148	G	6.0
32	2a	1000	G	6.0
1	2A	934	C	6.0
32	1a	1120	C	6.0
32	2a	1114	G	6.0
34	1c	193	TYR	6.0
32	1a	957	C	5.9
44	1m	56	LEU	5.9
6	2G	134	GLY	5.9
41	2j	34	VAL	5.9
1	2A	2157	C	5.9
6	2G	142	PRO	5.9
14	2S	34	HIS	5.9
44	1m	66	LEU	5.9
41	1j	39	PRO	5.9
50	2s	8	GLY	5.9
1	2A	2172	G	5.9
32	1a	1016	G	5.9
1	1A	1114	A	5.9
44	2m	13	LYS	5.9
32	2a	1004	U	5.9

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Mol	Chain	Res	Type	RSRZ
34	1c	57	ILE	5.9
32	1a	1012	G	5.9
41	2j	71	LEU	5.9
1	1A	1100	G	5.8
32	2a	1025	G	5.8
1	1A	2139	U	5.8
32	2a	1276	G	5.8
32	2a	1284	U	5.8
41	1j	96	ILE	5.8
38	2g	99	LEU	5.8
1	1A	2176	G	5.8
32	2a	1002	G	5.8
6	2G	39	ILE	5.8
32	1a	1013	A	5.8
50	1s	35	SER	5.8
7	2H	44	VAL	5.8
44	1m	105	THR	5.8
44	1m	104	ARG	5.8
1	1A	929	G	5.7
32	2a	923	G	5.7
50	1s	8	GLY	5.7
14	2S	37	ALA	5.7
32	2a	1279	C	5.7
1	2A	1133	A	5.7
40	1i	74	ILE	5.7
1	1A	2178	G	5.7
1	1A	2187	G	5.7
34	1c	102	ASN	5.7
32	1a	1285	C	5.7
38	2g	71	PRO	5.7
1	1A	2133	G	5.7
44	2m	100	GLY	5.7
1	2A	1152	G	5.7
1	1A	1127	U	5.7
38	1g	85	TYR	5.6
32	1a	1033	G	5.6
32	2a	1010	G	5.6
1	1A	682	G	5.6
32	1a	1278	C	5.6
34	2c	24	ALA	5.6
38	1g	2	ALA	5.6
1	2A	2180	G	5.6

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Mol	Chain	Res	Type	RSRZ
32	1a	983	A	5.6
32	1a	1036	G	5.6
7	2H	175	LYS	5.6
1	2A	2182	C	5.6
8	2I	77	LEU	5.6
1	1A	1108	G	5.6
40	2i	88	TYR	5.6
44	1m	63	THR	5.6
6	2G	135	LEU	5.5
32	1a	1006	C	5.5
32	1a	78	G	5.5
32	1a	1163	G	5.5
32	2a	1335	G	5.5
42	2k	22	HIS	5.5
32	2a	1013	A	5.5
32	1a	1115	C	5.5
32	2a	1286	G	5.5
32	1a	1102	C	5.5
38	2g	156	TRP	5.5
32	2a	985	C	5.5
32	2a	1252	C	5.5
32	1a	1200	C	5.5
44	2m	84	ILE	5.5
1	2A	2901	G	5.5
45	1n	60	SER	5.5
38	1g	152	ALA	5.5
1	1A	937	G	5.5
1	1A	2175	G	5.5
32	1a	1197	G	5.5
1	1A	1142	U	5.4
1	2A	1091	A	5.4
1	2A	1140	A	5.4
1	1A	1150	U	5.4
41	2j	94	VAL	5.4
48	1q	15	MET	5.4
32	1a	76	G	5.4
32	1a	968	C	5.4
8	2I	79	ILE	5.4
46	2o	89	GLY	5.4
1	2A	2153	U	5.4
1	1A	936	A	5.3
32	1a	75	C	5.3

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Mol	Chain	Res	Type	RSRZ
7	2H	24	VAL	5.3
32	2a	1255	G	5.3
34	2c	76	VAL	5.3
50	1s	39	THR	5.3
1	2A	1141	A	5.3
32	2a	1021	C	5.3
32	1a	1008	C	5.3
32	2a	1316	G	5.3
6	1G	80	PHE	5.3
1	1A	1933	A	5.3
32	2a	1225	C	5.3
34	1c	59	ARG	5.3
26	24	20	ASN	5.3
32	2a	1108	U	5.3
50	2s	83	HIS	5.3
32	2a	973	C	5.2
1	2A	2804	G	5.2
26	24	60	GLN	5.2
34	1c	88	ARG	5.2
40	1i	64	THR	5.2
1	1A	2168	G	5.2
6	2G	131	TYR	5.2
44	1m	18	ALA	5.2
1	2A	2904	C	5.2
1	2A	2191	A	5.2
32	1a	1103	G	5.2
1	2A	2178	G	5.2
32	2a	1008	C	5.2
41	2j	84	GLN	5.2
38	1g	125	MET	5.2
44	2m	67	GLU	5.1
32	1a	998	C	5.1
44	1m	64	TRP	5.1
44	1m	111	LYS	5.1
1	2A	1094	C	5.1
34	1c	103	VAL	5.1
32	1a	1146	C	5.1
44	2m	102	ARG	5.1
50	2s	3	ARG	5.1
44	1m	30	ALA	5.1
42	2k	43	SER	5.1
50	1s	33	THR	5.1

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Mol	Chain	Res	Type	RSRZ
34	1c	55	VAL	5.1
50	2s	45	VAL	5.1
40	1i	75	ASP	5.1
32	1a	1284	U	5.1
38	1g	71	PRO	5.1
48	1q	66	SER	5.1
6	1G	41	GLN	5.1
34	1c	101	LEU	5.0
32	2a	1163	G	5.0
1	1A	2128	C	5.0
1	1A	2159	C	5.0
44	2m	110	ARG	5.0
34	1c	66	VAL	5.0
1	2A	2137	G	5.0
32	1a	1206	G	5.0
1	1A	2129	C	5.0
34	2c	39	ILE	5.0
41	1j	37	PRO	5.0
1	2A	2145	G	5.0
32	2a	1212	C	5.0
34	2c	65	ALA	5.0
26	24	15	ILE	5.0
1	2A	1089	G	5.0
1	2A	1114	A	5.0
6	1G	44	GLY	5.0
1	1A	2124	C	5.0
32	1a	1121	G	5.0
42	2k	50	TYR	5.0
26	24	64	GLY	5.0
32	2a	1243	A	5.0
6	2G	49	ASP	4.9
32	2a	1012	G	4.9
35	2d	7	PRO	4.9
50	2s	10	PHE	4.9
1	1A	2174	G	4.9
40	2i	17	VAL	4.9
1	1A	1111	U	4.9
38	2g	80	VAL	4.9
32	2a	1001	G	4.9
32	2a	1282	G	4.9
32	2a	1244	C	4.9
40	1i	3	GLN	4.9

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Mol	Chain	Res	Type	RSRZ
6	2G	133	LEU	4.9
1	2A	1101	G	4.9
1	1A	2152	G	4.9
14	2S	33	LYS	4.9
32	1a	1341	C	4.9
32	2a	85	C	4.9
50	2s	34	TRP	4.9
32	2a	1285	C	4.9
41	1j	70	ARG	4.9
32	1a	1243	A	4.9
1	2A	302	C	4.8
34	1c	99	VAL	4.8
32	1a	1030	G	4.8
38	2g	37	ASN	4.8
40	1i	41	VAL	4.8
26	24	18	CYS	4.8
32	1a	1026	C	4.8
32	2a	1194	U	4.8
1	2A	933	A	4.8
1	1A	2125	G	4.8
38	2g	91	VAL	4.8
38	1g	98	SER	4.8
34	1c	87	LEU	4.8
1	1A	2901	G	4.8
32	2a	1007	C	4.8
1	1A	2154	G	4.8
32	1a	1107	G	4.8
32	1a	962	C	4.8
45	1n	32	SER	4.8
7	2H	25	LYS	4.8
41	2j	25	GLU	4.8
42	2k	42	TRP	4.8
32	1a	1268	A	4.8
32	1a	1004	U	4.8
33	2b	70	PHE	4.7
6	1G	88	ILE	4.7
11	2P	114	ILE	4.7
44	1m	46	LYS	4.7
34	1c	58	GLU	4.7
50	2s	70	LYS	4.7
52	1u	3	LYS	4.7
38	1g	35	LYS	4.7

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Mol	Chain	Res	Type	RSRZ
38	2g	112	PRO	4.7
32	1a	1212	C	4.7
1	2A	2902	G	4.7
32	2a	1077	G	4.7
32	2a	1197	G	4.7
32	2a	1323	U	4.7
32	1a	1277	G	4.7
50	1s	69	HIS	4.7
44	1m	114	ARG	4.7
11	2P	130	PHE	4.7
1	1A	2157	C	4.7
32	2a	1314	A	4.7
50	1s	79	THR	4.7
26	14	43	TYR	4.7
32	1a	1000	G	4.7
16	2U	76	TYR	4.7
41	2j	56	HIS	4.7
40	1i	21	PRO	4.7
1	1A	2802	A	4.7
1	2A	932	C	4.7
34	2c	104	GLN	4.7
38	1g	77	SER	4.7
32	1a	999	U	4.7
1	1A	695	C	4.7
32	1a	1279	C	4.7
1	2A	2155	A	4.7
7	2H	43	VAL	4.7
32	1a	996	G	4.7
32	1a	1157	G	4.7
1	2A	1093	A	4.7
1	2A	2136	G	4.6
41	2j	26	ALA	4.6
1	2A	2134	U	4.6
1	1A	930	C	4.6
1	1A	2156	A	4.6
42	2k	51	LYS	4.6
40	1i	37	PHE	4.6
1	2A	930	C	4.6
44	2m	114	ARG	4.6
1	1A	1130	A	4.6
32	2a	1269	A	4.6
32	2a	1481	A	4.6

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Mol	Chain	Res	Type	RSRZ
38	2g	88	PRO	4.6
21	2Z	97	GLU	4.6
32	2a	1009	C	4.6
34	2c	87	LEU	4.6
32	1a	1211	A	4.6
1	1A	2146	G	4.6
6	1G	135	LEU	4.6
1	2A	2171	U	4.6
26	14	4	GLY	4.6
40	2i	12	GLU	4.6
32	1a	72	C	4.6
50	2s	2	PRO	4.6
34	2c	155	GLY	4.6
32	1a	1269	A	4.6
40	1i	16	ARG	4.6
1	1A	1151	G	4.6
32	1a	1258	G	4.6
48	2q	65	ILE	4.5
32	1a	1252	C	4.5
32	2a	1158	A	4.5
41	2j	20	ALA	4.5
35	1d	7	PRO	4.5
1	1A	1139	U	4.5
6	1G	156	ASP	4.5
45	1n	33	VAL	4.5
32	2a	961	A	4.5
26	14	59	PHE	4.5
6	2G	159	VAL	4.5
1	2A	375	G	4.5
1	2A	2203	G	4.5
32	1a	995	A	4.5
38	2g	4	ARG	4.5
1	2A	2197	A	4.5
22	10	8	GLY	4.5
31	29	37	GLY	4.5
1	1A	1107	G	4.5
34	1c	77	ILE	4.5
34	2c	152	ILE	4.5
42	2k	45	GLY	4.5
41	1j	94	VAL	4.5
32	2a	1196	C	4.5
36	1e	118	ILE	4.5

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Mol	Chain	Res	Type	RSRZ
1	1A	2186	G	4.5
33	2b	101	MET	4.4
32	2a	1210	C	4.4
34	2c	206	GLU	4.4
32	2a	981	G	4.4
32	1a	1007	C	4.4
44	1m	13	LYS	4.4
38	1g	96	GLN	4.4
48	1q	16	GLN	4.4
32	1a	1256	G	4.4
34	2c	199	LYS	4.4
32	2a	1257	A	4.4
32	1a	1181	U	4.4
32	1a	1224	C	4.4
45	1n	59	ALA	4.4
1	2A	1130	A	4.4
6	2G	45	GLU	4.4
44	1m	87	TYR	4.4
32	2a	425	U	4.4
11	2P	115	LEU	4.4
32	1a	978	U	4.4
33	2b	19	HIS	4.4
34	2c	102	ASN	4.4
1	2A	2144	G	4.4
44	1m	29	ARG	4.4
34	2c	78	GLY	4.4
1	2A	2195	C	4.4
32	2a	998	C	4.4
35	2d	8	VAL	4.4
32	2a	1247	G	4.4
32	2a	1248	G	4.4
38	1g	95	ARG	4.4
40	1i	107	ARG	4.4
1	1A	2155	A	4.3
32	1a	972	A	4.3
1	2A	935	C	4.3
49	2r	46	GLU	4.3
33	2b	214	ILE	4.3
38	2g	32	ARG	4.3
1	2A	2168	G	4.3
44	2m	18	ALA	4.3
44	1m	107	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
40	1i	90	PRO	4.3
41	2j	23	ILE	4.3
44	1m	117	VAL	4.3
38	2g	155	ARG	4.3
42	1k	42	TRP	4.3
1	2A	1940	A	4.3
1	2A	2125	G	4.3
7	2H	4	ILE	4.3
41	2j	38	ILE	4.3
41	2j	87	THR	4.3
1	2A	944	A	4.3
26	14	66	SER	4.3
32	2a	1315	A	4.3
33	2b	215	LEU	4.3
38	1g	36	LYS	4.3
1	2A	1494	G	4.3
48	2q	45	HIS	4.3
7	2H	45	VAL	4.3
20	1Y	1	MET	4.3
32	1a	1106	A	4.3
34	2c	58	GLU	4.3
1	2A	2806	C	4.3
44	1m	102	ARG	4.3
44	2m	111	LYS	4.3
32	1a	952	A	4.3
40	1i	106	ALA	4.3
50	2s	84	GLY	4.3
32	2a	1128	C	4.3
32	2a	1246	C	4.3
1	2A	1107	G	4.3
32	1a	409	G	4.3
34	1c	89	GLU	4.2
32	2a	925	G	4.2
42	2k	32	ILE	4.2
26	14	61	ARG	4.2
42	2k	31	THR	4.2
32	1a	915	A	4.2
44	2m	57	ARG	4.2
35	2d	42	GLN	4.2
32	2a	84	A	4.2
1	2A	931	C	4.2
32	1a	1196	C	4.2

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Mol	Chain	Res	Type	RSRZ
42	2k	19	ALA	4.2
1	2A	303	C	4.2
32	2a	1195	A	4.2
6	1G	155	MET	4.2
42	2k	54	ARG	4.2
32	2a	422	G	4.2
32	1a	1257	A	4.2
38	1g	78	ARG	4.2
52	1u	14	TRP	4.2
48	1q	17	LYS	4.2
34	1c	69	HIS	4.2
1	1A	2902	G	4.2
32	1a	1127	G	4.2
1	1A	2160	C	4.2
1	1A	1098	C	4.2
1	2A	1132	G	4.2
1	2A	2900	A	4.2
32	1a	1156	G	4.2
32	1a	1208	C	4.2
32	2a	74	G	4.2
34	1c	67	THR	4.2
1	1A	2147	A	4.2
1	1A	2197	A	4.2
1	2A	936	A	4.2
44	2m	42	ALA	4.2
23	2l	81	LYS	4.2
52	2u	18	TYR	4.2
32	2a	1259	C	4.1
38	2g	70	LYS	4.1
40	1i	94	ALA	4.1
26	24	32	TYR	4.1
37	2f	65	VAL	4.1
32	2a	934	U	4.1
34	2c	56	ASP	4.1
32	2a	963	C	4.1
32	1a	1002	G	4.1
48	1q	69	LYS	4.1
34	2c	184	TYR	4.1
41	1j	5	ARG	4.1
1	1A	2322	A	4.1
40	2i	123	PRO	4.1
7	2H	103	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
32	1a	77	G	4.1
41	2j	70	ARG	4.1
1	2A	2813	C	4.1
32	1a	1112	C	4.1
5	1F	15	SER	4.1
32	1a	74	G	4.1
32	2a	931	G	4.1
26	14	3	GLU	4.1
34	1c	197	GLY	4.1
32	1a	1031	G	4.1
38	2g	96	GLN	4.1
1	1A	934	C	4.1
32	1a	1039	U	4.1
1	1A	1116	G	4.1
2	2B	5	C	4.1
32	1a	1158	A	4.1
40	1i	98	PRO	4.1
40	1i	42	ARG	4.1
26	24	42	PHE	4.1
32	1a	1314	A	4.1
32	2a	1113	A	4.1
38	1g	131	LYS	4.1
1	2A	937	G	4.1
32	1a	1320	G	4.1
6	1G	81	LYS	4.0
48	1q	98	LEU	4.0
50	2s	30	LEU	4.0
1	2A	1117	C	4.0
1	1A	2136	G	4.0
1	1A	2179	A	4.0
1	2A	2322	A	4.0
32	1a	1161	A	4.0
32	1a	1332	A	4.0
37	2f	6	VAL	4.0
40	2i	117	HIS	4.0
40	1i	128	ARG	4.0
1	1A	1121	C	4.0
1	2A	1116	G	4.0
7	2H	137	ASP	4.0
32	2a	989	G	4.0
41	2j	74	ILE	4.0
42	2k	21	ILE	4.0

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Mol	Chain	Res	Type	RSRZ
40	2i	89	ASN	4.0
41	1j	8	LEU	4.0
41	1j	58	ASP	4.0
48	2q	68	ARG	4.0
1	2A	203	G	4.0
6	2G	73	ALA	4.0
40	2i	102	LEU	4.0
32	1a	997	C	4.0
32	2a	958	C	4.0
32	1a	1077	G	4.0
41	1j	73	ASP	4.0
22	20	8	GLY	4.0
32	2a	1109	U	4.0
6	1G	90	LEU	4.0
32	2a	987	C	4.0
32	1a	1282	G	4.0
32	2a	991	U	4.0
34	2c	43	LEU	4.0
1	1A	939	C	4.0
32	1a	1190	C	4.0
48	1q	70	ARG	4.0
33	1b	227	GLY	4.0
1	1A	933	A	4.0
1	1A	2135	A	4.0
44	2m	17	VAL	3.9
41	1j	93	GLY	3.9
32	2a	1100	G	3.9
26	14	32	TYR	3.9
32	1a	1376	U	3.9
32	2a	969	U	3.9
37	2f	89	MET	3.9
32	2a	1148	C	3.9
38	2g	5	ARG	3.9
32	1a	1201	U	3.9
6	2G	89	GLY	3.9
32	1a	1159	G	3.9
50	1s	10	PHE	3.9
38	1g	26	PHE	3.9
50	1s	4	SER	3.9
50	2s	40	ILE	3.9
1	1A	1110	U	3.9
26	14	13	ARG	3.9

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Mol	Chain	Res	Type	RSRZ
32	1a	70	G	3.9
32	1a	1025	G	3.9
40	1i	20	ARG	3.9
1	1A	1141	A	3.9
44	1m	69	GLU	3.9
6	2G	34	LEU	3.9
50	2s	11	VAL	3.9
1	2A	1151	G	3.9
32	1a	1194	U	3.9
38	1g	76	ARG	3.9
48	2q	70	ARG	3.9
44	2m	82	MET	3.9
47	2p	79	VAL	3.9
41	1j	23	ILE	3.9
32	2a	990	G	3.9
40	1i	9	ARG	3.9
41	2j	17	ASP	3.9
32	1a	341	C	3.9
32	1a	986	C	3.9
1	1A	1122	A	3.9
1	2A	679	G	3.9
32	1a	1142	U	3.8
34	2c	183	ASP	3.8
32	2a	176	G	3.8
32	2a	957	C	3.8
34	2c	59	ARG	3.8
35	1d	36	ARG	3.8
40	1i	121	ARG	3.8
32	2a	1509	A	3.8
38	1g	32	ARG	3.8
1	1A	2200	C	3.8
32	1a	1342	A	3.8
32	2a	955	A	3.8
40	2i	62	TYR	3.8
40	1i	89	ASN	3.8
48	2q	18	THR	3.8
32	1a	1297	U	3.8
41	2j	27	ALA	3.8
32	2a	1145	C	3.8
40	2i	90	PRO	3.8
40	2i	3	GLN	3.8
44	1m	42	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
23	2l	2	SER	3.8
41	2j	72	VAL	3.8
1	2A	1100	G	3.8
1	2A	2670	G	3.8
32	1a	71	G	3.8
33	2b	42	ILE	3.8
32	1a	943	A	3.8
32	2a	516	A	3.8
44	1m	48	LEU	3.8
48	2q	43	LEU	3.8
35	2d	37	PRO	3.8
40	1i	95	LYS	3.8
7	2H	33	LEU	3.8
32	1a	990	G	3.8
32	1a	1122	G	3.8
32	2a	1187	U	3.8
32	2a	956	A	3.8
50	1s	76	PRO	3.8
1	2A	2324	C	3.8
32	1a	987	C	3.8
32	1a	1324	C	3.8
44	2m	7	VAL	3.8
44	2m	60	VAL	3.8
1	2A	1092	G	3.8
32	1a	980	G	3.8
32	2a	1164	G	3.8
38	2g	28	ASN	3.8
32	1a	1232	A	3.8
32	1a	1270	A	3.8
32	2a	953	A	3.8
1	2A	1156	A	3.7
35	2d	36	ARG	3.7
32	2a	86	U	3.7
32	2a	1143	G	3.7
33	2b	216	SER	3.7
1	2A	2160	C	3.7
40	2i	93	ARG	3.7
45	1n	22	THR	3.7
1	1A	2145	G	3.7
20	2Y	60	PHE	3.7
32	1a	1011	C	3.7
32	2a	421	G	3.7

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Mol	Chain	Res	Type	RSRZ
40	2i	21	PRO	3.7
34	1c	151	VAL	3.7
50	2s	53	ASN	3.7
35	1d	5	ILE	3.7
38	1g	151	TYR	3.7
41	1j	62	HIS	3.7
41	1j	87	THR	3.7
48	1q	68	ARG	3.7
33	2b	232	PRO	3.7
32	2a	924	A	3.7
1	2A	2196	C	3.7
40	1i	63	ILE	3.7
33	1b	232	PRO	3.7
40	2i	97	LYS	3.7
37	2f	61	LEU	3.7
44	2m	62	ASN	3.7
38	2g	154	TYR	3.7
44	1m	43	THR	3.7
38	1g	41	ARG	3.7
21	2Z	137	ILE	3.7
34	1c	3	ASN	3.7
6	2G	160	VAL	3.7
7	2H	26	VAL	3.7
6	1G	89	GLY	3.7
50	2s	68	GLY	3.7
26	24	8	LYS	3.7
1	1A	2180	G	3.7
20	2Y	6	HIS	3.7
35	1d	25	ARG	3.7
1	1A	2132	C	3.7
1	2A	1933	A	3.7
32	1a	937	A	3.7
32	1a	1299	C	3.7
34	2c	201	TYR	3.7
33	2b	37	ASN	3.7
34	2c	28	GLN	3.7
32	1a	989	G	3.6
32	2a	1127	G	3.6
32	2a	1287	G	3.6
14	2S	35	ILE	3.6
1	2A	2163	C	3.6
52	1u	18	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
44	1m	100	GLY	3.6
50	2s	48	THR	3.6
50	2s	13	ASP	3.6
32	1a	414	C	3.6
32	2a	1110	G	3.6
52	1u	7	ARG	3.6
33	1b	231	GLU	3.6
9	2N	25	ARG	3.6
45	1n	23	ARG	3.6
1	1A	2181	G	3.6
32	1a	931	G	3.6
34	1c	35	GLU	3.6
33	2b	210	SER	3.6
36	2e	20	GLN	3.6
48	2q	71	PHE	3.6
50	1s	14	HIS	3.6
16	2U	90	VAL	3.6
40	1i	12	GLU	3.6
50	2s	31	ILE	3.6
1	1A	2131	G	3.6
1	2A	2811	A	3.6
6	2G	75	LYS	3.6
50	2s	79	THR	3.6
32	1a	423	U	3.6
32	2a	1283	U	3.6
38	2g	125	MET	3.6
41	1j	54	PHE	3.6
32	1a	956	A	3.6
32	2a	1331	A	3.6
41	1j	25	GLU	3.6
38	2g	53	LYS	3.6
38	1g	90	GLU	3.6
50	2s	32	LYS	3.6
32	1a	422	G	3.6
32	2a	906	G	3.6
8	2I	82	ARG	3.6
34	1c	199	LYS	3.6
1	2A	1102	A	3.6
1	2A	925	G	3.6
34	1c	104	GLN	3.6
8	2I	81	VAL	3.5
32	1a	1182	C	3.5

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Mol	Chain	Res	Type	RSRZ
32	2a	1231	C	3.5
32	2a	916	A	3.5
32	2a	917	G	3.5
26	14	8	LYS	3.5
1	1A	1128	U	3.5
32	1a	1193	U	3.5
32	1a	1312	U	3.5
32	1a	1029	A	3.5
35	1d	6	GLY	3.5
35	1d	35	ARG	3.5
51	1t	102	GLY	3.5
48	1q	43	LEU	3.5
1	1A	1935	C	3.5
50	1s	9	VAL	3.5
44	1m	41	PRO	3.5
32	2a	962	C	3.5
50	1s	41	VAL	3.5
1	2A	353	A	3.5
4	2E	182	LEU	3.5
14	2S	26	LEU	3.5
41	1j	41	PRO	3.5
41	2j	54	PHE	3.5
32	1a	1353	G	3.5
50	1s	3	ARG	3.5
1	2A	2150	C	3.5
6	2G	46	ALA	3.5
32	1a	1170	A	3.5
32	2a	1075	A	3.5
40	2i	11	LYS	3.5
40	2i	54	ASP	3.5
34	2c	80	GLY	3.5
1	1A	1104	G	3.5
32	2a	976	G	3.5
32	2a	1159	G	3.5
32	1a	967	C	3.5
32	2a	1123	C	3.5
32	2a	1185	C	3.5
32	2a	1205	C	3.5
38	2g	52	GLU	3.5
40	1i	125	TYR	3.5
32	2a	960	U	3.5
41	2j	62	HIS	3.5

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Mol	Chain	Res	Type	RSRZ
44	2m	96	LEU	3.5
52	1u	21	TYR	3.5
32	1a	1147	G	3.5
32	2a	250	G	3.5
32	2a	907	G	3.5
32	2a	1067	G	3.5
47	1p	16	HIS	3.5
1	2A	2143	U	3.5
51	2t	102	GLY	3.5
40	2i	70	LYS	3.5
45	2n	60	SER	3.5
44	1m	25	ILE	3.5
1	1A	2195	C	3.5
44	1m	40	ASN	3.5
1	1A	944	A	3.5
32	1a	138	A	3.5
44	2m	101	GLN	3.5
41	1j	85	LEU	3.5
32	2a	341	C	3.4
32	1a	90	U	3.4
32	1a	1360	A	3.4
34	2c	66	VAL	3.4
41	2j	69	ASN	3.4
26	24	7	PRO	3.4
32	1a	963	C	3.4
32	1a	1205	C	3.4
32	1a	1032	U	3.4
1	1A	2191	A	3.4
32	1a	965	G	3.4
32	2a	1156	G	3.4
34	1c	63	ASN	3.4
41	1j	40	LEU	3.4
26	24	1	MET	3.4
32	1a	1432	A	3.4
32	1a	929	G	3.4
32	1a	1313	G	3.4
50	2s	49	ILE	3.4
32	1a	73	C	3.4
32	1a	930	U	3.4
32	2a	1129	A	3.4
33	2b	163	PHE	3.4
35	2d	39	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
44	1m	97	PRO	3.4
7	2H	62	LYS	3.4
34	1c	21	ARG	3.4
38	2g	89	MET	3.4
44	1m	109	THR	3.4
32	1a	960	U	3.4
34	1c	194	GLY	3.4
52	2u	6	ARG	3.4
32	1a	1301	A	3.4
32	2a	1140	A	3.4
32	2a	1480	A	3.4
26	24	9	LEU	3.4
34	2c	101	LEU	3.4
34	1c	123	GLN	3.4
32	1a	1219	C	3.4
35	1d	2	GLY	3.4
33	2b	206	ASP	3.4
1	2A	2668	A	3.4
32	2a	1027	A	3.4
34	1c	32	LEU	3.4
34	2c	103	VAL	3.4
38	2g	16	LEU	3.4
1	1A	928	G	3.4
32	1a	1203	G	3.4
32	2a	424	G	3.4
40	1i	78	LYS	3.4
41	1j	89	ASP	3.4
52	2u	9	ARG	3.4
1	1A	2161	C	3.4
32	1a	1001	G	3.4
32	1a	1199	C	3.4
32	2a	71	G	3.4
32	2a	1221	A	3.4
48	2q	17	LYS	3.4
38	2g	101	LEU	3.4
35	2d	4	TYR	3.4
41	2j	6	ILE	3.4
1	2A	1124	C	3.4
32	2a	1245	C	3.4
21	2Z	192	ALA	3.3
32	2a	995	A	3.3
38	1g	149	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
40	1i	104	ARG	3.3
50	1s	28	LYS	3.3
32	1a	1336	C	3.3
33	2b	190	THR	3.3
32	2a	1068	U	3.3
44	2m	14	ARG	3.3
1	2A	2198	C	3.3
32	2a	1317	C	3.3
34	1c	85	ARG	3.3
40	2i	69	GLY	3.3
1	1A	2177	G	3.3
1	1A	2805	G	3.3
32	1a	951	G	3.3
32	1a	988	G	3.3
1	1A	2190	A	3.3
1	2A	924	A	3.3
34	1c	110	ASN	3.3
7	2H	3	ARG	3.3
32	2a	75	C	3.3
34	2c	196	LEU	3.3
42	2k	27	ASN	3.3
1	1A	1143	A	3.3
32	1a	961	A	3.3
42	1k	43	SER	3.3
1	2A	2669	C	3.3
42	1k	30	VAL	3.3
44	1m	15	VAL	3.3
32	1a	1255	G	3.3
32	2a	1235	G	3.3
32	2a	977	C	3.3
1	2A	1105	U	3.3
32	2a	1181	U	3.3
28	26	39	TYR	3.3
1	2A	1118	A	3.3
17	2V	5	VAL	3.3
34	1c	68	VAL	3.3
1	2A	1587	G	3.3
41	2j	73	ASP	3.3
34	1c	190	ARG	3.3
44	1m	17	VAL	3.3
32	1a	1162	A	3.3
32	1a	1218	A	3.3

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Mol	Chain	Res	Type	RSRZ
32	2a	690	A	3.3
32	2a	974	A	3.3
32	2a	1230	A	3.3
32	2a	409	G	3.3
41	1j	45	ARG	3.3
1	1A	2182	C	3.3
26	24	43	TYR	3.3
40	2i	50	LEU	3.3
41	1j	90	LEU	3.3
45	1n	34	TYR	3.3
1	2A	1090	A	3.3
14	2S	87	PHE	3.3
32	1a	922	G	3.3
32	1a	1375	G	3.3
45	2n	14	PRO	3.3
32	2a	1372	C	3.3
7	2H	140	LYS	3.3
1	2A	2179	A	3.2
32	1a	1300	A	3.2
32	2a	1234	A	3.2
1	1A	2151	U	3.2
1	1A	2126	C	3.2
32	1a	92	G	3.2
32	1a	917	G	3.2
32	2a	1294	G	3.2
44	1m	96	LEU	3.2
6	2G	125	PHE	3.2
40	2i	53	VAL	3.2
35	1d	3	ARG	3.2
20	2Y	1	MET	3.2
41	1j	84	GLN	3.2
32	1a	936	A	3.2
32	1a	1038	A	3.2
32	1a	1131	U	3.2
34	1c	78	GLY	3.2
52	1u	12	LYS	3.2
1	1A	2199	C	3.2
32	1a	1145	C	3.2
41	2j	53	PRO	3.2
6	2G	47	LYS	3.2
20	2Y	46	LYS	3.2
32	1a	928	U	3.2

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Mol	Chain	Res	Type	RSRZ
32	1a	1140	A	3.2
38	2g	102	ARG	3.2
32	2a	1112	C	3.2
32	2a	1144	C	3.2
32	1a	1319	G	3.2
33	1b	228	GLY	3.2
32	1a	1311	A	3.2
6	1G	157	ILE	3.2
35	1d	43	HIS	3.2
1	1A	938	C	3.2
1	2A	942	C	3.2
1	2A	1166	C	3.2
21	2Z	51	ALA	3.2
50	1s	81	ARG	3.2
34	2c	144	SER	3.2
32	1a	1354	G	3.2
41	2j	55	LYS	3.2
4	2E	48	GLN	3.2
41	2j	37	PRO	3.2
1	2A	939	C	3.2
32	2a	1249	C	3.2
32	2a	1324	C	3.2
1	2A	202	G	3.2
1	1A	1940	A	3.2
32	2a	1378	C	3.2
32	1a	1108	U	3.2
32	2a	423	U	3.2
36	1e	6	PHE	3.2
38	2g	128	ALA	3.2
32	2a	993	A	3.2
34	1c	185	GLY	3.2
42	2k	29	ILE	3.2
32	1a	1028	C	3.2
34	2c	36	ASP	3.2
1	2A	2151	U	3.2
35	2d	13	ARG	3.2
32	1a	992	G	3.2
32	2a	554	G	3.2
40	1i	46	ALA	3.2
21	2Z	9	TYR	3.2
32	1a	1210	C	3.2
33	2b	23	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
38	2g	95	ARG	3.2
1	2A	1493	G	3.2
32	1a	68	C	3.1
36	1e	119	LEU	3.1
1	1A	1135	U	3.1
38	2g	87	VAL	3.1
38	1g	92	SER	3.1
38	2g	109	ASN	3.1
41	1j	44	VAL	3.1
44	1m	103	THR	3.1
1	1A	2900	A	3.1
32	1a	1213	G	3.1
32	1a	1351	G	3.1
32	2a	166	A	3.1
35	2d	35	ARG	3.1
1	2A	2485	C	3.1
32	2a	999	U	3.1
32	2a	1201	U	3.1
36	2e	75	THR	3.1
50	2s	54	GLY	3.1
1	2A	629	U	3.1
41	2j	61	GLU	3.1
32	1a	1335	G	3.1
32	2a	1206	G	3.1
50	1s	78	ARG	3.1
6	2G	112	PRO	3.1
44	1m	47	ASP	3.1
6	2G	148	MET	3.1
1	2A	1934	A	3.1
32	1a	970	U	3.1
42	2k	20	TYR	3.1
2	2B	79	C	3.1
32	1a	473	C	3.1
44	2m	48	LEU	3.1
32	2a	1121	G	3.1
38	2g	132	GLY	3.1
33	2b	234	PRO	3.1
42	2k	30	VAL	3.1
34	2c	21	ARG	3.1
42	2k	44	SER	3.1
33	2b	107	THR	3.1
32	2a	70	G	3.1

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Mol	Chain	Res	Type	RSRZ
44	1m	33	ALA	3.1
7	2H	123	PHE	3.1
21	2Z	146	ILE	3.1
44	1m	44	ARG	3.1
14	1S	51	ALA	3.1
32	2a	1099	C	3.1
21	2Z	23	LYS	3.1
21	2Z	155	LEU	3.1
1	2A	697	G	3.1
33	2b	201	ILE	3.1
4	2E	33	VAL	3.1
40	1i	65	VAL	3.1
34	2c	49	SER	3.1
6	2G	62	LEU	3.1
42	1k	19	ALA	3.1
50	1s	70	LYS	3.1
32	1a	973	C	3.1
36	2e	118	ILE	3.1
45	1n	29	ARG	3.1
7	2H	52	VAL	3.1
38	1g	31	MET	3.1
1	1A	1136	G	3.1
1	1A	2165	U	3.1
44	1m	24	GLY	3.1
34	1c	82	GLU	3.1
33	1b	96	ARG	3.1
32	1a	934	U	3.1
32	2a	1040	G	3.1
40	1i	57	GLY	3.1
44	2m	43	THR	3.1
40	1i	113	LYS	3.1
32	1a	1113	A	3.1
32	1a	1234	A	3.1
34	2c	3	ASN	3.0
40	1i	18	PHE	3.0
33	2b	8	LYS	3.0
40	2i	115	GLY	3.0
26	24	21	VAL	3.0
1	2A	304	G	3.0
32	1a	424	G	3.0
48	1q	45	HIS	3.0
1	2A	1112	A	3.0

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Mol	Chain	Res	Type	RSRZ
6	1G	42	GLY	3.0
32	2a	1432	A	3.0
38	2g	78	ARG	3.0
40	2i	85	LEU	3.0
1	2A	277	G	3.0
44	1m	50	GLU	3.0
1	1A	932	C	3.0
6	2G	79	ASN	3.0
32	1a	1101	C	3.0
34	2c	108	ASN	3.0
37	1f	6	VAL	3.0
8	1I	90	GLY	3.0
40	2i	107	ARG	3.0
41	1j	83	GLU	3.0
14	2S	38	GLN	3.0
1	1A	2184	C	3.0
2	2B	4	C	3.0
2	2B	117	G	3.0
40	1i	97	LYS	3.0
32	2a	915	A	3.0
38	2g	150	ALA	3.0
42	2k	97	ALA	3.0
47	2p	9	PHE	3.0
1	1A	1131	A	3.0
1	2A	1126	U	3.0
32	2a	79	G	3.0
38	1g	47	CYS	3.0
11	2P	116	GLY	3.0
52	2u	2	GLY	3.0
1	2A	2486	C	3.0
32	1a	1226	C	3.0
32	1a	340	A	3.0
32	1a	1023	U	3.0
32	1a	1010	G	3.0
32	1a	1286	G	3.0
32	2a	251	G	3.0
32	2a	943	A	3.0
32	2a	1069	U	3.0
32	2a	996	G	3.0
38	1g	86	GLN	3.0
6	1G	108	ASN	3.0
41	1j	27	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	1A	696	C	3.0
1	2A	368	A	3.0
50	2s	82	GLY	3.0
40	2i	36	TYR	3.0
52	2u	21	TYR	3.0
36	1e	40	ARG	3.0
44	2m	66	LEU	3.0
42	1k	39	PRO	3.0
33	1b	59	GLU	3.0
34	1c	81	GLY	3.0
50	1s	27	GLU	3.0
26	14	67	TYR	3.0
38	1g	100	ALA	3.0
32	1a	155	A	3.0
1	1A	2127	G	3.0
32	1a	1116	G	3.0
32	1a	1164	G	3.0
32	2a	1253	G	3.0
33	1b	70	PHE	3.0
42	2k	55	LYS	3.0
52	2u	17	THR	3.0
50	2s	47	HIS	3.0
1	1A	2123	U	3.0
1	2A	1127	U	3.0
34	2c	200	ALA	3.0
38	2g	3	ARG	3.0
1	1A	2167	C	3.0
6	2G	120	LEU	3.0
32	2a	908	C	3.0
25	23	46	ASN	3.0
1	2A	1103	G	2.9
50	1s	68	GLY	2.9
45	2n	19	ARG	2.9
52	1u	9	ARG	2.9
32	2a	933	U	2.9
32	2a	73	C	2.9
40	1i	33	PHE	2.9
6	1G	134	GLY	2.9
7	2H	51	ARG	2.9
39	2h	64	LYS	2.9
40	1i	55	ALA	2.9
1	2A	2142	G	2.9

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Mol	Chain	Res	Type	RSRZ
32	1a	91	G	2.9
46	2o	18	PHE	2.9
40	1i	93	ARG	2.9
32	2a	1102	C	2.9
40	2i	6	GLY	2.9
34	2c	72	LYS	2.9
44	2m	97	PRO	2.9
32	1a	1262	A	2.9
1	2A	2905	U	2.9
32	2a	1039	U	2.9
32	2a	1254	G	2.9
41	1j	55	LYS	2.9
50	1s	66	MET	2.9
32	1a	1191	C	2.9
32	2a	473	C	2.9
32	2a	1241	C	2.9
42	1k	31	THR	2.9
44	2m	109	THR	2.9
41	2j	95	GLU	2.9
32	1a	1283	U	2.9
11	2P	83	VAL	2.9
32	1a	1272	G	2.9
33	2b	17	PHE	2.9
38	1g	48	LYS	2.9
46	1o	21	ASP	2.9
1	2A	1157	G	2.9
32	2a	1030	G	2.9
32	2a	1265	G	2.9
32	2a	1313	G	2.9
48	2q	15	MET	2.9
34	1c	61	ALA	2.9
44	1m	106	ASN	2.9
38	1g	129	GLU	2.9
33	2b	98	LEU	2.9
42	1k	29	ILE	2.9
32	2a	902	C	2.9
45	1n	16	PHE	2.9
34	2c	110	ASN	2.9
44	2m	104	ARG	2.9
6	1G	120	LEU	2.9
50	1s	44	MET	2.9
50	1s	71	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
22	20	68	GLU	2.9
32	2a	912	C	2.9
32	2a	940	C	2.9
1	2A	2181	G	2.9
32	2a	1072	G	2.9
38	2g	82	GLY	2.9
1	2A	1254	A	2.9
33	1b	214	ILE	2.9
40	1i	19	LEU	2.9
24	22	46	GLN	2.9
21	2Z	93	ASP	2.9
6	2G	122	PRO	2.9
14	1S	52	SER	2.9
42	2k	40	ILE	2.9
44	2m	103	THR	2.9
1	1A	2137	G	2.9
2	2B	106	G	2.9
32	1a	69	G	2.9
32	1a	203	A	2.9
32	1a	941	G	2.9
32	2a	1240	G	2.9
33	1b	144	ARG	2.9
40	1i	62	TYR	2.9
40	1i	92	TYR	2.9
6	2G	154	GLY	2.9
33	1b	237	ALA	2.8
34	1c	28	GLN	2.8
42	2k	28	THR	2.8
14	2S	36	TYR	2.8
50	2s	50	ALA	2.8
1	1A	2169	G	2.8
1	2A	2162	G	2.8
8	1I	138	ILE	2.8
41	1j	63	PHE	2.8
26	24	38	LYS	2.8
1	2A	938	C	2.8
35	1d	38	TYR	2.8
36	2e	114	GLY	2.8
6	2G	87	PRO	2.8
26	24	49	PHE	2.8
37	1f	7	ASN	2.8
32	1a	950	C	2.8

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Mol	Chain	Res	Type	RSRZ
1	2A	1591	A	2.8
1	1A	2144	G	2.8
1	2A	1104	G	2.8
6	2G	81	LYS	2.8
32	1a	966	G	2.8
32	1a	1040	G	2.8
40	1i	102	LEU	2.8
33	1b	222	ILE	2.8
35	2d	43	HIS	2.8
40	1i	91	ASP	2.8
41	2j	18	ALA	2.8
1	2A	2156	A	2.8
6	1G	79	ASN	2.8
1	1A	1105	U	2.8
8	2I	70	GLU	2.8
32	2a	1023	U	2.8
41	1j	91	PRO	2.8
44	2m	50	GLU	2.8
1	1A	2166	C	2.8
32	1a	1249	C	2.8
32	2a	68	C	2.8
32	2a	1134	A	2.8
32	2a	1357	A	2.8
32	2a	1360	A	2.8
40	1i	103	THR	2.8
42	2k	41	THR	2.8
1	2A	1213	G	2.8
4	2E	186	GLY	2.8
38	1g	103	TRP	2.8
32	1a	1123	C	2.8
32	2a	1155	G	2.8
32	2a	1275	G	2.8
41	2j	30	SER	2.8
44	1m	84	ILE	2.8
48	1q	71	PHE	2.8
32	2a	1131	U	2.8
34	1c	29	TYR	2.8
34	2c	17	ASP	2.8
43	2l	72	GLY	2.8
34	2c	75	VAL	2.8
32	2a	988	G	2.8
40	1i	43	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
49	2r	20	ALA	2.8
32	1a	370	A	2.8
32	1a	1027	A	2.8
8	1I	129	THR	2.8
18	2W	5	ALA	2.8
32	2a	673	C	2.8
1	1A	2141	G	2.8
32	1a	1015	G	2.8
32	2a	753	G	2.8
32	2a	1122	G	2.8
38	2g	93	PRO	2.8
21	2Z	156	LYS	2.8
21	2Z	138	GLU	2.8
32	2a	1239	U	2.8
33	1b	221	LEU	2.8
50	2s	20	LEU	2.8
8	2I	78	THR	2.8
38	1g	132	GLY	2.8
32	1a	1259	C	2.8
50	2s	76	PRO	2.8
52	1u	22	ARG	2.8
40	2i	110	GLU	2.7
29	17	1	MET	2.7
32	2a	1256	G	2.7
7	2H	96	ALA	2.7
8	1I	46	ALA	2.7
34	1c	198	VAL	2.7
36	2e	6	PHE	2.7
37	2f	63	TYR	2.7
38	2g	63	LYS	2.7
44	1m	5	ALA	2.7
50	1s	74	PHE	2.7
33	1b	201	ILE	2.7
36	2e	120	THR	2.7
1	1A	1109	C	2.7
32	1a	1095	C	2.7
32	1a	969	U	2.7
32	1a	1119	U	2.7
1	1A	2675	G	2.7
14	2S	51	ALA	2.7
32	2a	1353	G	2.7
35	1d	185	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	2A	5	A	2.7
1	2A	700	A	2.7
6	2G	58	GLN	2.7
25	23	43	ILE	2.7
35	2d	40	PRO	2.7
1	1A	2163	C	2.7
38	1g	87	VAL	2.7
7	2H	18	GLU	2.7
1	2A	1975	G	2.7
32	1a	1202	G	2.7
32	2a	1117	G	2.7
32	2a	1204	G	2.7
1	2A	1555	A	2.7
38	1g	17	VAL	2.7
1	2A	1554	C	2.7
1	2A	1592	C	2.7
32	1a	48	C	2.7
32	2a	1479	C	2.7
40	1i	126	SER	2.7
41	1j	28	ARG	2.7
41	2j	41	PRO	2.7
48	1q	100	LYS	2.7
5	2F	169	ASN	2.7
34	1c	111	LEU	2.7
1	1A	1939	A	2.7
1	2A	1573	A	2.7
8	2I	84	GLY	2.7
35	1d	23	GLY	2.7
38	2g	6	ARG	2.7
44	1m	32	GLU	2.7
1	2A	1158	U	2.7
32	2a	1326	C	2.7
44	1m	34	LEU	2.7
6	1G	131	TYR	2.7
45	2n	7	ILE	2.7
52	1u	24	ARG	2.7
32	2a	202	A	2.7
1	1A	1089	G	2.7
32	2a	1033	G	2.7
32	2a	1180	G	2.7
32	2a	1213	G	2.7
37	2f	21	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	1A	1146	U	2.7
1	1A	2198	C	2.7
32	1a	148	C	2.7
32	1a	1344	C	2.7
35	2d	6	GLY	2.7
7	2H	141	VAL	2.7
40	1i	114	TYR	2.7
1	1A	1216	G	2.7
6	2G	109	VAL	2.7
26	24	68	ARG	2.7
40	2i	18	PHE	2.7
32	1a	1143	G	2.7
32	2a	707	U	2.7
52	2u	22	ARG	2.7
3	2D	156	ALA	2.7
34	2c	105	GLU	2.7
41	1j	6	ILE	2.7
1	2A	1553	A	2.7
7	2H	19	VAL	2.7
1	1A	1123	U	2.7
6	2G	158	ALA	2.7
32	1a	156	A	2.7
50	2s	67	VAL	2.7
51	1t	70	SER	2.7
32	1a	935	U	2.7
40	2i	75	ASP	2.7
1	2A	1215	G	2.7
8	2I	72	LEU	2.7
21	2Z	157	LEU	2.7
32	2a	1103	G	2.7
41	1j	7	LYS	2.7
6	1G	87	PRO	2.7
40	1i	67	GLY	2.7
26	24	6	HIS	2.7
40	2i	5	TYR	2.7
41	1j	59	SER	2.7
1	1A	1541	A	2.7
1	2A	678	A	2.7
6	2G	108	ASN	2.7
38	1g	84	ASN	2.7
32	1a	1192	C	2.7
32	2a	449	C	2.7

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Mol	Chain	Res	Type	RSRZ
47	1p	80	PHE	2.7
1	2A	2763	G	2.7
32	1a	1126	G	2.7
32	1a	1305	G	2.7
41	1j	61	GLU	2.7
34	2c	33	LEU	2.6
40	1i	47	LEU	2.6
32	2a	180	A	2.6
32	2a	1376	U	2.6
32	2a	208	C	2.6
7	2H	59	ARG	2.6
34	1c	126	ARG	2.6
38	2g	25	ALA	2.6
38	2g	153	HIS	2.6
40	1i	66	ARG	2.6
48	2q	44	ALA	2.6
38	2g	103	TRP	2.6
38	2g	68	ASN	2.6
1	1A	2130	U	2.6
6	2G	38	VAL	2.6
14	2S	49	VAL	2.6
32	1a	1105	U	2.6
33	2b	203	GLY	2.6
1	2A	1095	A	2.6
32	2a	369	A	2.6
33	2b	187	LEU	2.6
1	2A	1125	C	2.6
26	14	65	ASP	2.6
32	1a	1223	G	2.6
32	2a	1343	G	2.6
50	2s	65	ASN	2.6
35	1d	45	GLN	2.6
47	2p	75	ARG	2.6
8	2I	138	ILE	2.6
1	1A	1091	A	2.6
1	2A	941	A	2.6
14	2S	112	PHE	2.6
32	1a	1063	A	2.6
32	1a	1220	A	2.6
32	2a	1170	A	2.6
8	2I	142	VAL	2.6
32	2a	1124	C	2.6

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Mol	Chain	Res	Type	RSRZ
44	2m	80	ARG	2.6
1	2A	1624	U	2.6
2	2B	98	G	2.6
32	1a	1188	G	2.6
32	2a	1203	G	2.6
32	1a	147	A	2.6
32	2a	1186	A	2.6
32	1a	451	C	2.6
32	1a	1141	C	2.6
39	1h	28	ALA	2.6
32	1a	825	U	2.6
1	2A	1463	G	2.6
32	1a	1337	G	2.6
34	2c	120	VAL	2.6
38	1g	34	GLY	2.6
1	2A	2135	A	2.6
42	2k	104	GLN	2.6
32	2a	1224	C	2.6
44	1m	11	ARG	2.6
35	2d	41	GLY	2.6
8	1I	139	GLN	2.6
38	1g	30	ILE	2.6
1	1A	2815	G	2.6
1	2A	2360	G	2.6
32	1a	1172	G	2.6
40	2i	119	ALA	2.6
32	1a	413	C	2.6
32	1a	948	C	2.6
32	2a	1171	C	2.6
40	1i	39	GLY	2.6
1	1A	2171	U	2.6
32	1a	1347	U	2.6
45	1n	4	LYS	2.6
46	1o	17	ARG	2.6
6	1G	49	ASP	2.6
8	2I	65	ALA	2.6
33	2b	204	ASN	2.6
42	1k	38	ASN	2.6
44	2m	61	GLU	2.6
49	1r	22	VAL	2.6
50	1s	73	GLU	2.6
1	2A	204	A	2.6

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Mol	Chain	Res	Type	RSRZ
11	2P	113	LYS	2.6
32	2a	905	G	2.6
32	2a	1325	G	2.6
40	2i	27	THR	2.6
32	1a	1246	C	2.6
38	2g	38	LEU	2.6
15	2T	84	GLN	2.6
32	1a	1295	U	2.6
35	2d	38	TYR	2.6
6	1G	45	GLU	2.6
38	2g	129	GLU	2.6
4	2E	34	VAL	2.6
40	2i	22	GLY	2.6
48	1q	20	THR	2.6
1	2A	1511	G	2.6
1	2A	2871	G	2.6
32	1a	911	G	2.6
32	1a	1207	A	2.6
32	2a	69	G	2.6
32	1a	958	C	2.6
41	1j	47	PHE	2.6
32	1a	1290	U	2.6
44	2m	75	ALA	2.6
6	1G	137	GLU	2.6
44	1m	45	VAL	2.6
40	1i	29	ASN	2.6
49	1r	43	PHE	2.5
38	2g	152	ALA	2.5
1	2A	1977	U	2.5
1	2A	2202	G	2.5
32	2a	980	G	2.5
32	2a	992	G	2.5
32	2a	1293	G	2.5
33	2b	99	GLY	2.5
33	1b	213	LEU	2.5
39	2h	35	ILE	2.5
8	1I	105	HIS	2.5
31	29	2	LYS	2.5
49	2r	43	PHE	2.5
38	2g	7	ALA	2.5
32	1a	1289	U	2.5
32	2a	978	U	2.5

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Mol	Chain	Res	Type	RSRZ
32	2a	1162	A	2.5
49	1r	40	LEU	2.5
1	2A	9	G	2.5
1	2A	267	G	2.5
34	2c	202	ILE	2.5
21	2Z	7	ALA	2.5
40	2i	20	ARG	2.5
26	14	64	GLY	2.5
38	1g	135	VAL	2.5
50	1s	22	LEU	2.5
26	24	37	SER	2.5
33	2b	222	ILE	2.5
45	2n	35	ARG	2.5
1	1A	1094	C	2.5
20	1Y	92	ASN	2.5
32	1a	450	C	2.5
34	2c	29	TYR	2.5
32	2a	1370	G	2.5
32	2a	1375	G	2.5
40	1i	96	LEU	2.5
32	1a	1104	U	2.5
32	2a	1217	U	2.5
38	2g	57	GLU	2.5
50	1s	42	PRO	2.5
26	14	63	TYR	2.5
1	1A	1129	A	2.5
1	2A	1131	A	2.5
28	26	42	TRP	2.5
32	1a	1209	A	2.5
32	1a	1378	C	2.5
32	1a	1480	A	2.5
34	2c	74	GLY	2.5
42	2k	17	GLY	2.5
32	2a	65	G	2.5
32	2a	67	G	2.5
33	1b	233	SER	2.5
34	2c	20	SER	2.5
21	2Z	8	TYR	2.5
27	25	60	VAL	2.5
45	2n	4	LYS	2.5
6	2G	94	LEU	2.5
6	2G	93	THR	2.5

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Mol	Chain	Res	Type	RSRZ
44	1m	116	THR	2.5
1	2A	1574	A	2.5
1	2A	2132	C	2.5
1	1A	2173	G	2.5
32	2a	1169	G	2.5
36	2e	94	ALA	2.5
44	2m	28	ALA	2.5
32	2a	1119	U	2.5
6	2G	145	THR	2.5
38	2g	26	PHE	2.5
34	2c	89	GLU	2.5
41	1j	99	LYS	2.5
1	1A	2324	C	2.5
1	2A	2204	C	2.5
32	1a	1306	A	2.5
26	14	56	VAL	2.5
34	2c	195	VAL	2.5
35	2d	133	VAL	2.5
38	1g	101	LEU	2.5
38	2g	149	ARG	2.5
41	2j	49	VAL	2.5
33	2b	140	HIS	2.5
1	1A	697	G	2.5
1	2A	1134	G	2.5
38	2g	74	GLU	2.5
1	1A	2196	C	2.5
7	2H	128	PRO	2.5
32	1a	824	C	2.5
32	1a	1099	C	2.5
32	1a	1331	A	2.5
32	1a	1334	C	2.5
32	2a	897	A	2.5
32	2a	1063	A	2.5
32	2a	1098	C	2.5
32	2a	1262	A	2.5
32	2a	1318	C	2.5
50	2s	14	HIS	2.5
32	1a	1217	U	2.5
32	2a	1363	U	2.5
40	2i	16	ARG	2.5
1	2A	1167	G	2.5
17	2V	40	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
32	1a	1343	G	2.5
32	1a	1348	G	2.5
32	2a	1125	G	2.5
33	2b	207	ALA	2.5
38	1g	150	ALA	2.5
42	2k	46	GLY	2.5
44	1m	23	TYR	2.5
1	1A	1934	A	2.5
1	2A	2777	A	2.5
7	2H	124	GLU	2.5
34	1c	152	ILE	2.5
33	2b	137	ARG	2.5
50	1s	64	GLU	2.5
6	2G	65	GLY	2.5
47	2p	78	GLY	2.5
50	2s	9	VAL	2.5
8	2I	83	ALA	2.5
47	1p	38	TYR	2.5
21	2Z	149	SER	2.5
1	1A	2164	C	2.4
32	2a	415	C	2.4
32	2a	1208	C	2.4
32	1a	369	A	2.4
32	1a	942	A	2.4
32	1a	993	A	2.4
41	1j	22	LYS	2.4
32	2a	959	U	2.4
34	1c	184	TYR	2.4
50	1s	80	TYR	2.4
35	2d	115	ARG	2.4
47	1p	76	GLN	2.4
1	1A	2804	G	2.4
6	1G	34	LEU	2.4
1	2A	836	C	2.4
1	2A	1564	G	2.4
32	2a	918	C	2.4
32	2a	949	G	2.4
32	2a	1111	C	2.4
32	2a	1115	C	2.4
50	2s	75	ALA	2.4
1	2A	1153	U	2.4
15	2T	93	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
32	2a	1073	U	2.4
11	2P	94	GLU	2.4
33	1b	223	ILE	2.4
44	1m	39	ILE	2.4
40	1i	117	HIS	2.4
20	2Y	59	GLY	2.4
8	1I	82	ARG	2.4
38	1g	68	ASN	2.4
48	1q	18	THR	2.4
32	2a	1271	A	2.4
50	1s	2	PRO	2.4
33	2b	38	GLY	2.4
34	1c	196	LEU	2.4
40	2i	40	LEU	2.4
6	2G	117	PHE	2.4
16	2U	89	GLU	2.4
41	2j	83	GLU	2.4
47	1p	69	THR	2.4
1	2A	2817	U	2.4
35	1d	40	PRO	2.4
33	1b	187	LEU	2.4
50	1s	60	VAL	2.4
1	2A	335	G	2.4
1	2A	926	G	2.4
33	1b	148	TYR	2.4
45	1n	58	LYS	2.4
7	2H	47	GLU	2.4
38	1g	42	ILE	2.4
39	2h	77	GLU	2.4
44	2m	40	ASN	2.4
47	2p	74	LEU	2.4
50	2s	71	LEU	2.4
1	2A	1150	U	2.4
6	2G	147	ASP	2.4
1	2A	1590	A	2.4
38	1g	154	TYR	2.4
32	1a	1276	G	2.4
32	1a	1329	G	2.4
33	2b	52	GLU	2.4
10	2O	57	VAL	2.4
17	2V	14	VAL	2.4
38	1g	53	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
38	2g	62	PHE	2.4
33	2b	33	TYR	2.4
14	2S	39	ILE	2.4
32	1a	1148	C	2.4
32	2a	1097	C	2.4
32	2a	1350	C	2.4
33	1b	226	ARG	2.4
33	2b	217	ARG	2.4
44	1m	71	ARG	2.4
32	1a	167	A	2.4
32	1a	1250	A	2.4
32	2a	349	A	2.4
7	2H	17	VAL	2.4
32	1a	1153	G	2.4
32	2a	1202	G	2.4
38	1g	89	MET	2.4
33	1b	55	PHE	2.4
38	1g	54	THR	2.4
43	2l	71	PRO	2.4
11	2P	117	GLU	2.4
38	1g	33	ASP	2.4
32	1a	1171	C	2.4
32	2a	1154	C	2.4
40	1i	26	VAL	2.4
41	2j	7	LYS	2.4
41	2j	93	GLY	2.4
52	2u	4	GLY	2.4
1	2A	699	A	2.4
48	1q	64	PRO	2.4
34	1c	160	ALA	2.4
44	2m	51	ALA	2.4
1	2A	1572	G	2.4
1	2A	2815	G	2.4
32	1a	454	G	2.4
32	2a	1031	G	2.4
41	1j	80	LYS	2.4
49	2r	76	LEU	2.4
8	1I	145	VAL	2.4
38	1g	62	PHE	2.4
40	2i	37	PHE	2.4
32	1a	1318	C	2.4
32	1a	1479	C	2.4

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Mol	Chain	Res	Type	RSRZ
26	14	53	GLU	2.4
1	1A	1553	A	2.4
34	1c	108	ASN	2.4
7	2H	72	ILE	2.4
40	1i	99	LEU	2.4
8	2I	145	VAL	2.4
44	1m	54	VAL	2.4
32	2a	1041	G	2.4
33	1b	209	ARG	2.4
50	2s	43	GLU	2.4
1	2A	1149	C	2.4
1	2A	2200	C	2.4
50	2s	80	TYR	2.4
35	1d	21	LEU	2.4
32	1a	1481	A	2.3
32	2a	994	A	2.3
47	1p	75	ARG	2.3
14	2S	40	ILE	2.3
28	26	41	PRO	2.3
32	1a	1362	G	2.3
32	2a	1362	G	2.3
40	2i	81	ILE	2.3
32	2a	914	C	2.3
26	14	1	MET	2.3
8	1I	73	GLU	2.3
32	2a	448	A	2.3
32	2a	1024	A	2.3
18	1W	5	ALA	2.3
21	2Z	62	PRO	2.3
32	2a	689	U	2.3
38	2g	98	SER	2.3
31	29	4	ARG	2.3
44	2m	71	ARG	2.3
6	2G	67	LYS	2.3
32	1a	905	G	2.3
32	2a	672	G	2.3
40	1i	127	LYS	2.3
4	2E	35	GLN	2.3
40	1i	110	GLU	2.3
8	2I	91	SER	2.3
32	1a	974	A	2.3
32	1a	1322	A	2.3

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Mol	Chain	Res	Type	RSRZ
38	2g	22	LEU	2.3
38	2g	127	ALA	2.3
33	1b	101	MET	2.3
35	2d	33	MET	2.3
50	1s	47	HIS	2.3
50	2s	57	HIS	2.3
35	2d	34	GLU	2.3
45	2n	8	GLU	2.3
1	2A	1144	G	2.3
1	2A	1467	G	2.3
1	2A	1931	G	2.3
1	2A	2167	C	2.3
1	2A	2199	C	2.3
4	2E	2	LYS	2.3
8	2I	107	VAL	2.3
40	2i	44	VAL	2.3
1	2A	1541	A	2.3
32	1a	946	A	2.3
32	2a	896	A	2.3
32	2a	901	A	2.3
32	2a	1165	A	2.3
32	2a	1218	A	2.3
50	1s	21	GLU	2.3
40	1i	31	GLN	2.3
41	1j	43	ARG	2.3
45	2n	3	ARG	2.3
8	1I	107	VAL	2.3
32	2a	1296	C	2.3
32	2a	1126	G	2.3
36	1e	93	PRO	2.3
38	1g	13	GLN	2.3
41	2j	33	GLN	2.3
51	1t	55	ILE	2.3
36	2e	8	GLU	2.3
38	1g	52	GLU	2.3
39	2h	116	LYS	2.3
1	1A	2170	G	2.3
1	2A	379	G	2.3
6	1G	133	LEU	2.3
32	2a	935	U	2.3
45	2n	61	TRP	2.3
32	1a	1183	A	2.3

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Mol	Chain	Res	Type	RSRZ
32	1a	1238	A	2.3
38	1g	128	ALA	2.3
50	2s	74	PHE	2.3
34	2c	119	ARG	2.3
20	2Y	4	LYS	2.3
21	2Z	199	LYS	2.3
41	2j	64	GLU	2.3
42	2k	71	LYS	2.3
32	2a	149	C	2.3
38	1g	97	GLN	2.3
5	2F	21	ALA	2.3
34	2c	177	THR	2.3
38	1g	69	VAL	2.3
32	1a	65	G	2.3
32	1a	89	G	2.3
32	1a	1024	A	2.3
32	1a	1293	G	2.3
32	2a	207	G	2.3
48	1q	14	LYS	2.3
48	2q	67	LYS	2.3
47	1p	15	PRO	2.3
14	2S	110	LEU	2.3
26	24	39	CYS	2.3
34	1c	113	ALA	2.3
35	1d	10	ARG	2.3
32	2a	1219	C	2.3
32	2a	1345	C	2.3
44	1m	53	VAL	2.3
26	14	54	GLY	2.3
36	1e	92	LYS	2.3
40	1i	115	GLY	2.3
47	1p	37	GLY	2.3
40	1i	54	ASP	2.3
45	2n	54	PRO	2.3
1	2A	159	G	2.3
2	2B	72	G	2.3
32	2a	1116	G	2.3
32	2a	1301	A	2.3
32	2a	1320	G	2.3
50	2s	5	LEU	2.3
5	1F	17	ARG	2.3
38	2g	77	SER	2.3

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Mol	Chain	Res	Type	RSRZ
34	2c	82	GLU	2.3
5	2F	32	LEU	2.3
37	1f	61	LEU	2.3
52	1u	23	PRO	2.3
17	2V	4	ILE	2.3
1	2A	701	A	2.3
32	2a	543	A	2.3
32	2a	751	A	2.3
32	2a	1106	A	2.3
32	2a	1207	A	2.3
1	2A	378	G	2.2
32	2a	76	G	2.2
35	1d	41	GLY	2.2
6	1G	40	ASN	2.2
37	2f	7	ASN	2.2
32	2a	1397	U	2.2
40	2i	83	ARG	2.2
52	1u	6	ARG	2.2
32	1a	1144	C	2.2
32	2a	1028	C	2.2
35	1d	37	PRO	2.2
1	1A	1591	A	2.2
8	1I	128	LEU	2.2
1	1A	2183	G	2.2
1	2A	1912	G	2.2
32	1a	1139	G	2.2
38	2g	131	LYS	2.2
34	1c	120	VAL	2.2
32	1a	1317	C	2.2
45	1n	61	TRP	2.2
34	1c	183	ASP	2.2
33	1b	93	VAL	2.2
36	1e	75	THR	2.2
40	2i	33	PHE	2.2
42	1k	47	VAL	2.2
50	1s	65	ASN	2.2
1	1A	1217	G	2.2
1	1A	1912	G	2.2
1	2A	2667	U	2.2
32	1a	1125	G	2.2
32	2a	965	G	2.2
34	1c	155	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
38	1g	64	GLN	2.2
40	2i	43	ALA	2.2
1	1A	2904	C	2.2
40	2i	79	LEU	2.2
34	1c	142	MET	2.2
37	2f	8	ILE	2.2
6	2G	130	ASN	2.2
41	1j	24	VAL	2.2
44	2m	53	VAL	2.2
1	2A	1683	A	2.2
7	2H	46	GLU	2.2
34	2c	2	GLY	2.2
34	2c	109	PRO	2.2
1	1A	1624	U	2.2
32	2a	1347	U	2.2
21	2Z	150	LEU	2.2
34	1c	91	LEU	2.2
40	1i	40	LEU	2.2
1	1A	898	G	2.2
8	2I	88	ILE	2.2
32	2a	1200	C	2.2
26	24	30	GLU	2.2
37	1f	63	TYR	2.2
50	2s	22	LEU	2.2
7	2H	41	MET	2.2
34	2c	207	VAL	2.2
40	2i	78	LYS	2.2
42	2k	47	VAL	2.2
1	1A	2142	G	2.2
14	2S	47	THR	2.2
47	2p	76	GLN	2.2
38	1g	73	MET	2.2
43	2l	102	ARG	2.2
32	1a	994	A	2.2
32	2a	927	A	2.2
32	2a	928	U	2.2
40	1i	109	VAL	2.2
42	1k	32	ILE	2.2
50	1s	62	ILE	2.2
21	2Z	29	TYR	2.2
41	1j	32	ALA	2.2
1	1A	1633	C	2.2

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Mol	Chain	Res	Type	RSRZ
1	2A	1223	C	2.2
26	24	61	ARG	2.2
32	1a	449	C	2.2
34	1c	73	PRO	2.2
32	1a	320	G	2.2
32	1a	1235	G	2.2
32	2a	1036	G	2.2
32	2a	1051	G	2.2
41	1j	42	THR	2.2
33	2b	97	TRP	2.2
35	2d	5	ILE	2.2
44	2m	54	VAL	2.2
34	2c	185	GLY	2.2
41	1j	52	GLY	2.2
1	1A	1555	A	2.2
1	2A	1129	A	2.2
34	2c	100	ALA	2.2
36	1e	94	ALA	2.2
38	1g	83	ALA	2.2
47	1p	17	TYR	2.2
6	2G	55	LYS	2.2
36	1e	64	ARG	2.2
8	1I	81	VAL	2.2
26	24	33	VAL	2.2
32	1a	520	C	2.2
32	1a	1034	C	2.2
22	20	28	GLY	2.2
32	1a	96	G	2.2
32	2a	460	G	2.2
5	2F	101	LEU	2.2
43	2l	120	TYR	2.2
32	2a	1267	A	2.2
44	2m	16	ASP	2.2
8	2I	144	VAL	2.2
33	1b	15	VAL	2.2
41	2j	48	THR	2.2
32	1a	1302	C	2.2
32	2a	1190	C	2.2
3	2D	119	ALA	2.2
8	1I	42	SER	2.2
17	2V	3	ALA	2.2
33	2b	221	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
36	2e	21	ALA	2.2
38	2g	18	TYR	2.2
1	1A	378	G	2.2
1	1A	2205	G	2.2
21	2Z	88	PHE	2.2
32	2a	32	G	2.2
32	2a	571	G	2.2
32	2a	1044	G	2.2
32	2a	1369	G	2.2
36	1e	38	GLN	2.2
50	1s	45	VAL	2.2
33	1b	16	HIS	2.2
38	2g	76	ARG	2.2
42	1k	41	THR	2.2
49	2r	49	LYS	2.2
52	1u	8	THR	2.2
8	2I	140	LEU	2.1
40	2i	114	TYR	2.1
1	1A	698	C	2.1
1	1A	943	C	2.1
1	2A	2562	C	2.1
21	2Z	128	VAL	2.1
25	23	12	PRO	2.1
4	2E	145	LYS	2.1
1	1A	1572	G	2.1
1	2A	289	G	2.1
32	1a	753	G	2.1
32	2a	91	G	2.1
40	1i	79	LEU	2.1
41	1j	69	ASN	2.1
46	2o	22	THR	2.1
49	2r	51	LEU	2.1
33	2b	218	ALA	2.1
36	1e	45	PHE	2.1
41	1j	11	PHE	2.1
49	1r	29	PHE	2.1
3	2D	228	PRO	2.1
6	1G	39	ILE	2.1
26	14	37	SER	2.1
32	1a	1350	C	2.1
32	2a	1429	C	2.1
34	2c	88	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
41	1j	49	VAL	2.1
26	14	17	GLY	2.1
1	2A	1625	A	2.1
32	1a	1294	G	2.1
36	2e	47	LYS	2.1
40	2i	95	LYS	2.1
47	1p	12	LYS	2.1
47	1p	42	ARG	2.1
33	1b	68	ILE	2.1
38	1g	50	ILE	2.1
37	1f	67	MET	2.1
38	2g	31	MET	2.1
1	2A	548	U	2.1
1	2A	1063	C	2.1
6	1G	152	LEU	2.1
32	1a	1035	U	2.1
32	1a	1352	C	2.1
32	2a	1118	U	2.1
32	2a	1264	C	2.1
46	2o	21	ASP	2.1
4	1E	46	ALA	2.1
9	2N	130	HIS	2.1
34	1c	6	HIS	2.1
44	2m	87	TYR	2.1
11	2P	124	LYS	2.1
50	1s	34	TRP	2.1
39	2h	61	VAL	2.1
42	1k	48	ILE	2.1
1	1A	681	G	2.1
1	2A	1939	A	2.1
1	2A	2205	G	2.1
1	2A	2211	G	2.1
2	2B	61	G	2.1
32	1a	1273	G	2.1
32	2a	614	G	2.1
32	2a	929	G	2.1
46	1o	20	GLY	2.1
47	2p	49	LEU	2.1
2	2B	6	C	2.1
32	1a	86	U	2.1
33	1b	163	PHE	2.1
33	2b	226	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
36	2e	40	ARG	2.1
44	1m	51	ALA	2.1
35	1d	8	VAL	2.1
38	2g	113	GLU	2.1
6	1G	2	PRO	2.1
34	1c	164	ARG	2.1
40	2i	42	ARG	2.1
1	1A	2811	A	2.1
5	2F	22	ALA	2.1
32	1a	151	G	2.1
32	1a	554	G	2.1
1	1A	2185	C	2.1
2	1B	5	C	2.1
8	1I	144	VAL	2.1
32	1a	1154	C	2.1
5	2F	134	GLY	2.1
26	14	60	GLN	2.1
34	1c	177	THR	2.1
34	2c	84	ILE	2.1
24	12	1	MET	2.1
50	1s	72	GLY	2.1
48	2q	64	PRO	2.1
21	2Z	63	ASP	2.1
1	1A	924	A	2.1
32	1a	1509	A	2.1
32	2a	942	A	2.1
32	2a	1321	A	2.1
32	1a	150	C	2.1
33	2b	111	ARG	2.1
50	2s	66	MET	2.1
38	2g	105	VAL	2.1
33	2b	40	HIS	2.1
42	1k	95	ILE	2.1
1	1A	941	A	2.1
1	2A	370	A	2.1
32	1a	168	U	2.1
1	2A	10	G	2.1
1	2A	1214	G	2.1
1	2A	1971	G	2.1
1	2A	2816	G	2.1
32	2a	795	C	2.1
32	2a	1034	C	2.1

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Mol	Chain	Res	Type	RSRZ
32	2a	1130	C	2.1
26	14	30	GLU	2.1
32	2a	1482	G	2.1
41	1j	95	GLU	2.1
34	1c	54	ARG	2.1
45	1n	26	ARG	2.1
19	2X	1	MET	2.1
1	2A	2892	A	2.1
32	2a	1029	A	2.1
32	2a	1220	A	2.1
32	2a	1300	A	2.1
34	2c	23	TYR	2.1
40	1i	119	ALA	2.1
52	2u	12	LYS	2.1
7	2H	49	VAL	2.1
46	1o	27	VAL	2.1
4	2E	81	ILE	2.1
32	2a	941	G	2.1
35	1d	134	ASP	2.1
51	1t	101	GLY	2.1
34	1c	107	GLN	2.1
15	2T	40	THR	2.1
35	1d	179	GLU	2.1
44	1m	108	ARG	2.1
40	1i	84	ALA	2.1
50	1s	77	THR	2.1
32	1a	166	A	2.1
32	2a	1281	A	2.1
42	2k	48	ILE	2.1
41	2j	10	GLY	2.1
32	2a	1371	C	2.1
33	2b	16	HIS	2.1
6	1G	153	ARG	2.0
6	2G	91	ARG	2.0
1	2A	276	G	2.0
8	2I	66	GLU	2.0
12	2Q	105	GLU	2.0
34	2c	85	ARG	2.0
38	1g	102	ARG	2.0
32	1a	1072	G	2.0
33	1b	225	ALA	2.0
41	2j	81	THR	2.0

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Mol	Chain	Res	Type	RSRZ
14	1S	58	LEU	2.0
16	2U	74	LEU	2.0
42	2k	98	LEU	2.0
1	2A	651	A	2.0
12	2Q	123	HIS	2.0
26	24	51	ASP	2.0
32	2a	1085	A	2.0
33	2b	48	MET	2.0
34	2c	79	ARG	2.0
35	1d	13	ARG	2.0
44	2m	64	TRP	2.0
51	1t	100	ILE	2.0
1	1A	1493	G	2.0
1	1A	2162	G	2.0
1	2A	1189	G	2.0
2	2B	116	G	2.0
32	1a	1180	G	2.0
32	2a	975	U	2.0
7	2H	152	ARG	2.0
35	2d	45	GLN	2.0
1	2A	971	A	2.0
8	2I	89	TYR	2.0
33	2b	165	VAL	2.0
38	2g	100	ALA	2.0
50	1s	19	VAL	2.0
1	2A	2814	C	2.0
32	1a	1111	C	2.0
32	2a	599	C	2.0
51	1t	54	LYS	2.0
34	2c	83	ARG	2.0
35	1d	132	ARG	2.0
1	1A	2905	U	2.0
1	2A	923	U	2.0
1	2A	2170	G	2.0
32	1a	1287	G	2.0
32	2a	89	G	2.0
32	2a	833	G	2.0
32	2a	903	G	2.0
34	2c	35	GLU	2.0
41	1j	34	VAL	2.0
4	1E	61	ARG	2.0
6	2G	144	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
33	1b	29	ALA	2.0
36	2e	119	LEU	2.0
38	1g	39	ALA	2.0
44	1m	2	ALA	2.0
8	1I	50	ARG	2.0
20	2Y	73	ARG	2.0
32	2a	1238	A	2.0
46	2o	88	ARG	2.0
20	2Y	56	PRO	2.0
32	2a	1344	C	2.0
21	1Z	202	GLU	2.0
32	2a	211	U	2.0
48	2q	16	GLN	2.0
25	23	11	SER	2.0
34	2c	154	SER	2.0
33	1b	39	ILE	2.0
34	1c	84	ILE	2.0
36	2e	17	ALA	2.0
47	1p	70	ALA	2.0
1	1A	927	G	2.0
1	1A	1463	G	2.0
1	1A	1524	G	2.0
1	2A	921	G	2.0
26	24	17	GLY	2.0
32	2a	954	G	2.0
52	2u	16	GLY	2.0
4	2E	74	PRO	2.0
1	2A	1629	A	2.0
1	1A	935	C	2.0
1	2A	33	C	2.0
32	2a	451	C	2.0
26	24	13	ARG	2.0
35	2d	21	LEU	2.0
37	2f	90	VAL	2.0
41	2j	85	LEU	2.0
42	1k	80	VAL	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column

labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	5MC	1A	1963	21/22	0.96	0.18	37,53,70,100	0
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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	2A	3105	1/1	0.34	0.36	88,88,88,88	0
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	1a	1851	1/1	0.54	0.53	84,84,84,84	0
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	2a	1703	1/1	0.64	0.57	84,84,84,84	0
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	2a	1789	1/1	0.69	0.67	79,79,79,79	0
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
53	MG	1a	1831	1/1	0.73	0.29	110,110,110,110	0
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	2a	1777	1/1	0.75	0.51	91,91,91,91	0
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	2A	3325	1/1	0.77	0.51	69,69,69,69	0
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	1A	3146	1/1	0.79	0.34	62,62,62,62	0
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	1A	3754	1/1	0.80	0.25	54,54,54,54	0
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	ZN	2n	102	1/1	0.81	0.12	205,205,205,205	0
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	2A	3121	1/1	0.83	0.17	70,70,70,70	0
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	1a	1734	1/1	0.84	0.39	86,86,86,86	0
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	1a	1710	1/1	0.84	0.77	86,86,86,86	0
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	1D	307	1/1	0.85	0.40	53,53,53,53	0
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	1a	1766	1/1	0.86	0.54	70,70,70,70	0
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	11	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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	1A	3420	1/1	0.87	0.30	66,66,66,66	0
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	2A	3335	1/1	0.88	0.20	95,95,95,95	0
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	1E	307	1/1	0.88	0.29	38,38,38,38	0
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	1A	3069	1/1	0.89	0.44	63,63,63,63	0
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	1A	3825	1/1	0.89	0.19	55,55,55,55	0
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	2A	3369	1/1	0.90	0.14	79,79,79,79	0
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	2a	1841	1/1	0.90	0.53	58,58,58,58	0
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	2I	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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	2A	3297	1/1	0.91	0.21	70,70,70,70	0
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	2A	3055	1/1	0.91	0.28	78,78,78,78	0
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	2A	3319	1/1	0.92	0.24	99,99,99,99	0
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	2A	3253	1/1	0.92	0.16	78,78,78,78	0
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	1U	201	1/1	0.92	0.28	58,58,58,58	0
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	1A	3532	1/1	0.93	0.22	82,82,82,82	0
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	1A	3573	1/1	0.93	0.16	67,67,67,67	0
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	2A	3060	1/1	0.93	0.09	112,112,112,112	0
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	2A	3178	1/1	0.94	0.17	96,96,96,96	0
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	1A	3143	1/1	0.94	0.09	69,69,69,69	0
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	1A	3780	1/1	0.94	0.41	74,74,74,74	0
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	1A	3822	1/1	0.95	0.21	25,25,25,25	0
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	2A	3176	1/1	0.95	0.25	70,70,70,70	0
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	2A	3410	1/1	0.95	0.16	88,88,88,88	0
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	1a	1862	1/1	0.95	0.16	87,87,87,87	0
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	1A	3397	1/1	0.96	0.26	61,61,61,61	0
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	1A	3123	1/1	0.96	0.13	68,68,68,68	0
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	1a	1728	1/1	0.96	0.18	78,78,78,78	0
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	1a	1833	1/1	0.97	0.13	67,67,67,67	0
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	2A	3169	1/1	0.97	0.43	61,61,61,61	0
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	2A	3078	1/1	0.97	0.40	61,61,61,61	0
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	1A	3378	1/1	0.98	0.14	52,52,52,52	0
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	1A	3078	1/1	0.98	0.26	91,91,91,91	0
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	1A	3111	1/1	0.98	0.20	81,81,81,81	0
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

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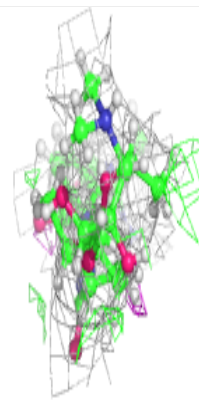
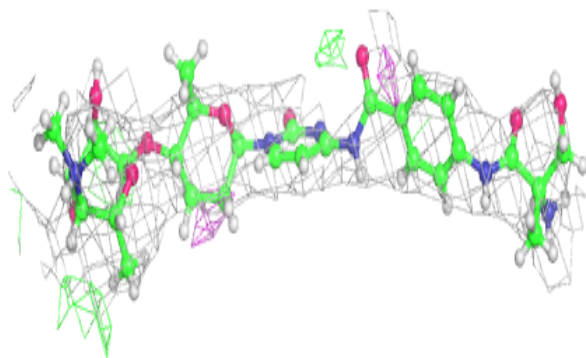
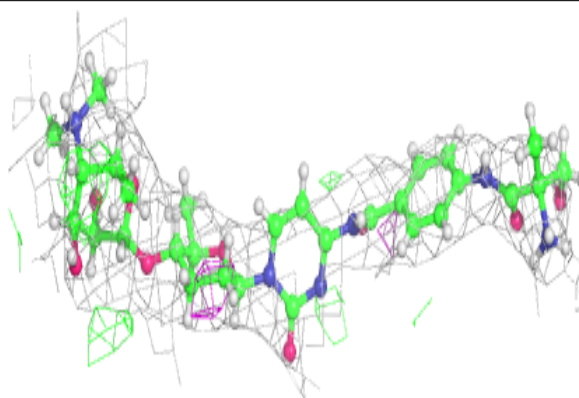
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	1A	3036	1/1	0.99	0.14	57,57,57,57	0
53	MG	1A	3274	1/1	0.99	0.24	56,56,56,56	0
53	MG	1A	3345	1/1	0.99	0.23	47,47,47,47	0
53	MG	1A	3149	1/1	1.00	0.20	55,55,55,55	0
53	MG	1A	3056	1/1	1.00	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.

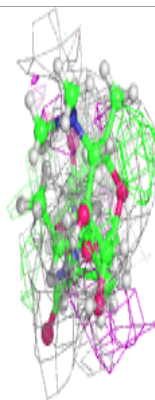
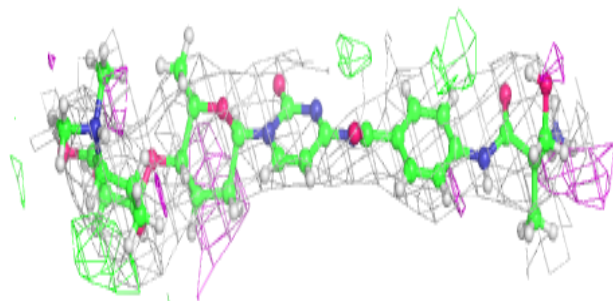
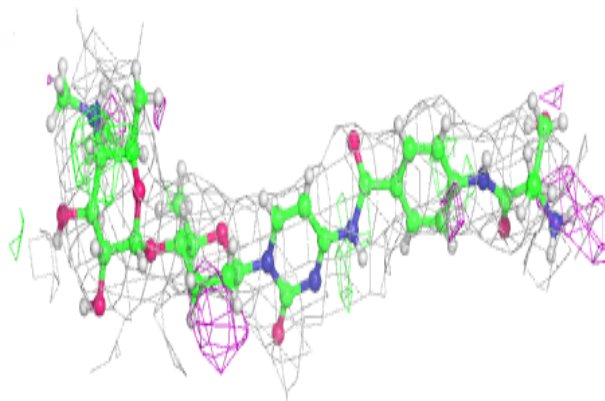
Electron density around FSD 2A 3553:

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



Electron density around 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.