



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 12, 2021 – 11:30 AM EDT

PDB ID : 7MD7
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with triphenylphosphonium analog of chloramphenicol CAM-C4-TPP and protein Y (YfiA) at 2.80Å resolution
Authors : Chen, C.-W.; Pavlova, J.A.; Lukianov, D.A.; Tereshchenkov, A.G.; Makarov, G.I.; Khairullina, Z.Z.; Tashlitsky, V.N.; Paleskava, A.; Konevega, A.L.; Bogdanov, A.A.; Osterman, I.A.; Sumbatyan, N.V.; Polikanov, Y.S.
Deposited on : 2021-04-03
Resolution : 2.80 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	:	2.18
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)	:	2.18

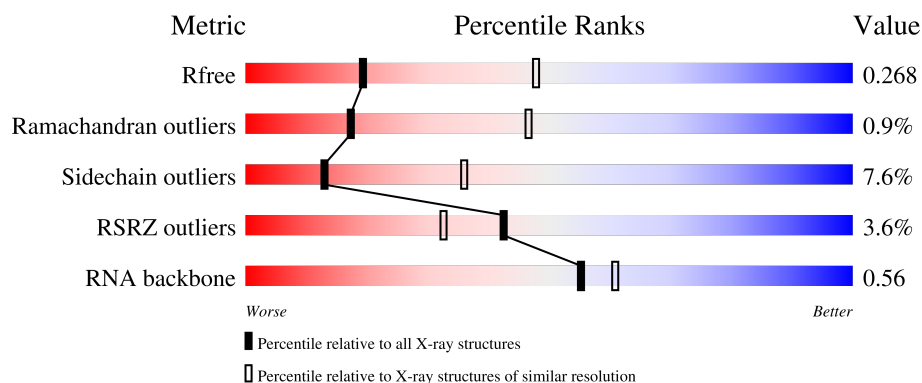
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)
RNA backbone	3102	1227 (3.10-2.50)

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

Mol	Chain	Length	Quality of chain
1	1A	2915	<div> <div>%</div> <div> <div></div> <div>83%</div> <div>15%</div> <div>.</div> </div> </div>
1	2A	2915	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>17%</div> <div>.</div> </div> </div>
2	1B	121	<div> <div></div> <div> <div></div> <div>91%</div> <div>8%</div> <div>.</div> </div> </div>
2	2B	121	<div> <div>%</div> <div> <div></div> <div>88%</div> <div>11%</div> <div>.</div> </div> </div>
3	1D	276	<div> <div></div> <div> <div></div> <div>93%</div> <div>6%</div> <div>.</div> </div> </div>





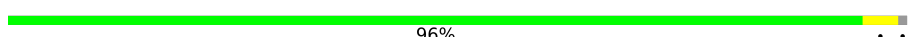
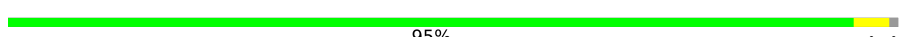




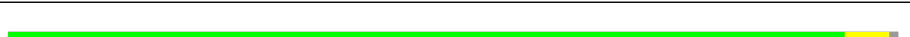


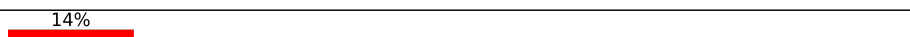
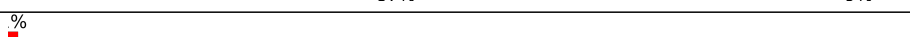
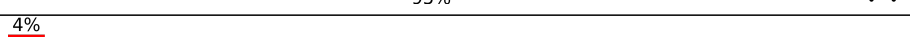
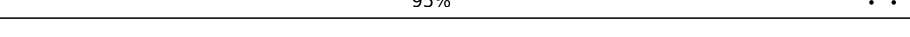

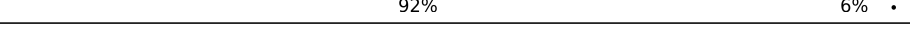
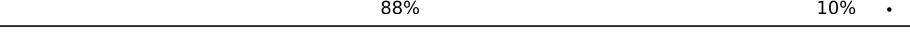



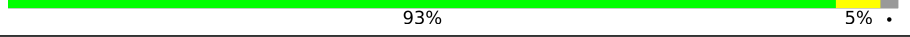
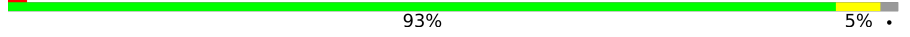
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Mol	Chain	Length	Quality of chain
3	2D	276	<div> <div>4%</div> <div>96%</div> <div>.</div> </div>
4	1E	206	<div> <div></div> <div>94%</div> <div>5% .</div> </div>
4	2E	206	<div> <div>%</div> <div>93%</div> <div>6% .</div> </div>
5	1F	210	<div> <div></div> <div>89%</div> <div>8% .</div> </div>
5	2F	210	<div> <div></div> <div>90%</div> <div>7% .</div> </div>
6	1G	182	<div> <div>%</div> <div>92%</div> <div>8% .</div> </div>
6	2G	182	<div> <div>18%</div> <div>90%</div> <div>9% .</div> </div>
7	1H	180	<div> <div>%</div> <div>91%</div> <div>6% .</div> </div>
7	2H	180	<div> <div>3%</div> <div>85%</div> <div>11% .</div> </div>
8	1I	148	<div> <div>%</div> <div>88%</div> <div>11% .</div> </div>
8	2I	148	<div> <div>2%</div> <div>91%</div> <div>7% ..</div> </div>
9	1N	140	<div> <div></div> <div>95%</div> <div>5%</div> </div>
9	2N	140	<div> <div>%</div> <div>99%</div> <div>.</div> </div>
10	1O	122	<div> <div></div> <div>96%</div> <div>.</div> </div>
10	2O	122	<div> <div></div> <div>96%</div> <div>.</div> </div>
11	1P	150	<div> <div></div> <div>95%</div> <div>. .</div> </div>
11	2P	150	<div> <div>3%</div> <div>95%</div> <div>5% .</div> </div>
12	1Q	141	<div> <div></div> <div>94%</div> <div>6% .</div> </div>
12	2Q	141	<div> <div>2%</div> <div>94%</div> <div>6%</div> </div>
13	1R	118	<div> <div></div> <div>92%</div> <div>8%</div> </div>
13	2R	118	<div> <div>3%</div> <div>95%</div> <div>5%</div> </div>
14	1S	112	<div> <div></div> <div>93%</div> <div>. . .</div> </div>
14	2S	112	<div> <div>7%</div> <div>90%</div> <div>8% .</div> </div>
15	1T	146	<div> <div>%</div> <div>86%</div> <div>. 10%</div> </div>
15	2T	146	<div> <div></div> <div>85%</div> <div>5% 10%</div> </div>

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Mol	Chain	Length	Quality of chain
16	1U	118	 91% 8% .
16	2U	118	 2% 92% 7% .
17	1V	101	 93% 6% .
17	2V	101	 92% 8% .
18	1W	113	 96% . .
18	2W	113	 95% . .
19	1X	96	 90% 9% .
19	2X	96	 % 92% 7% .
20	1Y	110	 % 91% 6% .
20	2Y	110	 4% 90% 7% .
21	1Z	206	 94% 5% .
21	2Z	206	 6% 90% 7% .
22	10	85	 87% . 9%
22	20	85	 14% 87% . 9%
23	11	98	 % 95% . .
23	21	98	 4% 95% . .
24	12	72	 90% 7% .
24	22	72	 92% 6% .
25	13	60	 88% 10% .
25	23	60	 88% 10% .
26	14	71	 % 80% 17% .
26	24	71	 18% 85% 10% . .
27	15	60	 93% 5% .
27	25	60	 2% 93% 5% .
28	16	54	 91% 7% .

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

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Mol	Chain	Length	Quality of chain
41	1j	105	
41	2j	105	
42	1k	129	
42	2k	129	
43	1l	132	
43	2l	132	
44	1m	126	
44	2m	126	
45	1n	61	
45	2n	61	
46	1o	89	
46	2o	89	
47	1p	88	
47	2p	88	
48	1q	105	
48	2q	105	
49	1r	88	
49	2r	88	
50	1s	93	
50	2s	93	
51	1t	106	
51	2t	106	
52	1u	27	
52	2u	27	
53	1y	113	

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Mol	Chain	Length	Quality of chain
53	2y	113	<div> <div>46%</div> <div>79%</div> <div>6%</div> <div>15%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	19	103	-	-	-	X
54	MG	1A	3075	-	-	-	X
54	MG	1A	4015	-	-	-	X
54	MG	1P	203	-	-	-	X
54	MG	2A	3074	-	-	-	X
54	MG	2A	3131	-	-	-	X
54	MG	2A	3435	-	-	-	X
54	MG	2A	3488	-	-	-	X
54	MG	2A	3512	-	-	-	X
54	MG	2A	3519	-	-	-	X
54	MG	2A	3646	-	-	-	X
54	MG	2A	3736	-	-	-	X
54	MG	2D	303	-	-	-	X
54	MG	2Q	202	-	-	-	X
54	MG	2V	201	-	-	-	X
54	MG	2a	3011	-	-	-	X

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 298171 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1A	2872	Total	C	N	O	P	0	0	0
			61869	27540	11574	19884	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
			1076	687	186	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 a protein called Ribosome-associated inhibitor A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1y	97	Total	C	N	O	S	0	0	0
			764	478	144	139	3			
53	2y	96	Total	C	N	O	S	0	0	0
			749	468	141	137	3			

- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	1A	1054	Total	Mg	0	0
			1054	1054		
54	1B	27	Total	Mg	0	0
			27	27		
54	1D	17	Total	Mg	0	0
			17	17		
54	1E	6	Total	Mg	0	0
			6	6		
54	1F	15	Total	Mg	0	0
			15	15		
54	1G	4	Total	Mg	0	0
			4	4		
54	1H	2	Total	Mg	0	0
			2	2		
54	1N	4	Total	Mg	0	0
			4	4		
54	1O	1	Total	Mg	0	0
			1	1		
54	1P	5	Total	Mg	0	0
			5	5		
54	1Q	5	Total	Mg	0	0
			5	5		
54	1R	6	Total	Mg	0	0
			6	6		
54	1S	1	Total	Mg	0	0
			1	1		
54	1T	6	Total	Mg	0	0
			6	6		
54	1U	8	Total	Mg	0	0
			8	8		
54	1V	5	Total	Mg	0	0
			5	5		
54	1W	4	Total	Mg	0	0
			4	4		
54	1Z	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	10	7	Total 7	Mg 7	0	0
54	11	5	Total 5	Mg 5	0	0
54	13	5	Total 5	Mg 5	0	0
54	14	1	Total 1	Mg 1	0	0
54	15	7	Total 7	Mg 7	0	0
54	16	1	Total 1	Mg 1	0	0
54	17	4	Total 4	Mg 4	0	0
54	18	1	Total 1	Mg 1	0	0
54	19	3	Total 3	Mg 3	0	0
54	1a	279	Total 279	Mg 279	0	0
54	1b	1	Total 1	Mg 1	0	0
54	1d	5	Total 5	Mg 5	0	0
54	1e	2	Total 2	Mg 2	0	0
54	1f	2	Total 2	Mg 2	0	0
54	1g	3	Total 3	Mg 3	0	0
54	1h	2	Total 2	Mg 2	0	0
54	1i	1	Total 1	Mg 1	0	0
54	1k	1	Total 1	Mg 1	0	0
54	1l	2	Total 2	Mg 2	0	0
54	1m	1	Total 1	Mg 1	0	0
54	1n	3	Total 3	Mg 3	0	0

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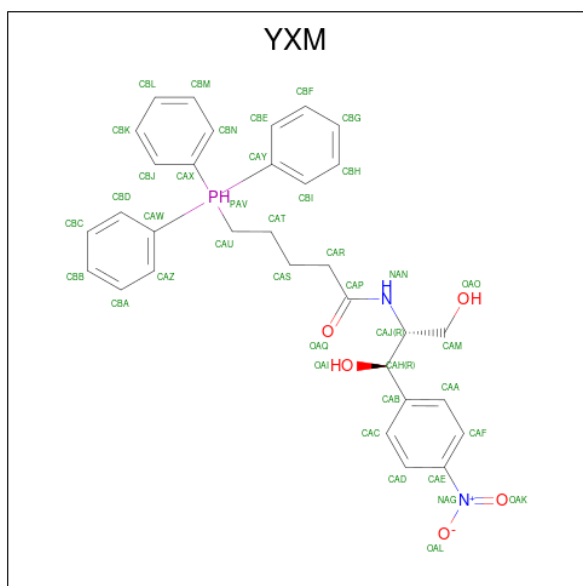
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	1o	2	Total 2	Mg 2	0	0
54	1t	1	Total 1	Mg 1	0	0
54	1y	4	Total 4	Mg 4	0	0
54	2A	757	Total 757	Mg 757	0	0
54	2B	19	Total 19	Mg 19	0	0
54	2D	12	Total 12	Mg 12	0	0
54	2E	6	Total 6	Mg 6	0	0
54	2F	3	Total 3	Mg 3	0	0
54	2G	3	Total 3	Mg 3	0	0
54	2I	1	Total 1	Mg 1	0	0
54	2N	1	Total 1	Mg 1	0	0
54	2O	2	Total 2	Mg 2	0	0
54	2P	2	Total 2	Mg 2	0	0
54	2Q	3	Total 3	Mg 3	0	0
54	2R	3	Total 3	Mg 3	0	0
54	2T	3	Total 3	Mg 3	0	0
54	2V	3	Total 3	Mg 3	0	0
54	2W	2	Total 2	Mg 2	0	0
54	2X	2	Total 2	Mg 2	0	0
54	2Y	1	Total 1	Mg 1	0	0
54	20	2	Total 2	Mg 2	0	0

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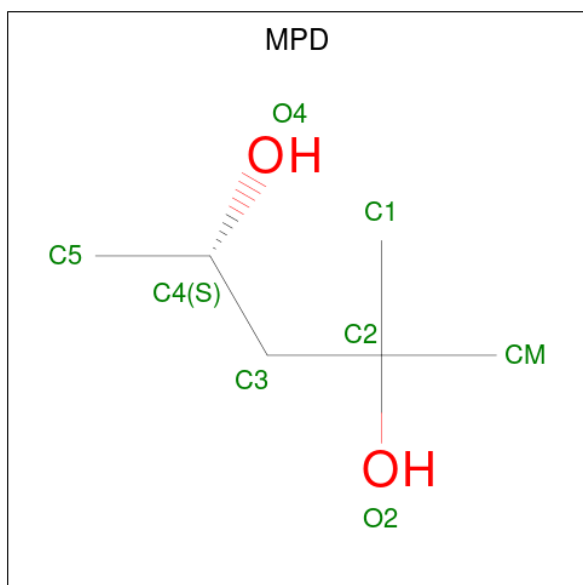
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
54	21	2	Total Mg 2 2	0	0
54	23	2	Total Mg 2 2	0	0
54	25	1	Total Mg 1 1	0	0
54	27	2	Total Mg 2 2	0	0
54	28	2	Total Mg 2 2	0	0
54	2a	200	Total Mg 200 200	0	0
54	2e	2	Total Mg 2 2	0	0
54	2f	1	Total Mg 1 1	0	0
54	2j	1	Total Mg 1 1	0	0
54	2n	1	Total Mg 1 1	0	0
54	2t	1	Total Mg 1 1	0	0

- Molecule 55 is N-[(1R,2R)-1,3-dihydroxy-1-(4-nitrophenyl)propan-2-yl]-5-(triphenyl-lambda 5 -phosphanyl)pentanamide (three-letter code: YXM) (formula: C₃₂H₃₅N₂O₅P).



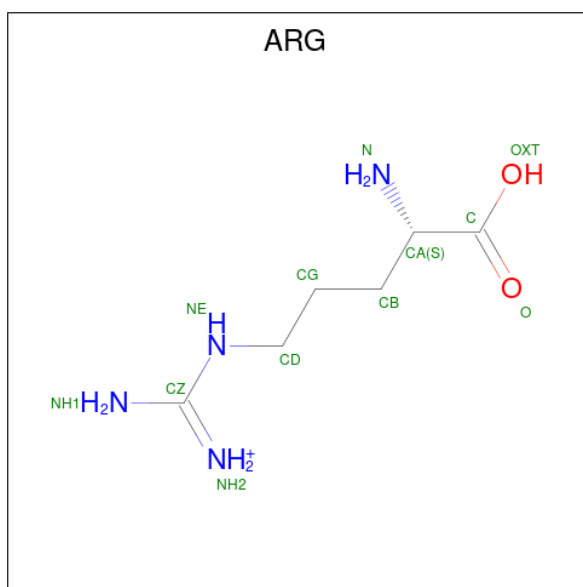
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
55	1A	1	Total	C	N	O	P	0	0
			40	32	2	5	1		
55	2A	1	Total	C	N	O	P	0	0
			40	32	2	5	1		

- Molecule 56 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	1A	1	Total	C	O	0	0
			8	6	2		
56	1T	1	Total	C	O	0	0
			8	6	2		
56	18	1	Total	C	O	0	0
			8	6	2		
56	1a	1	Total	C	O	0	0
			8	6	2		
56	2A	1	Total	C	O	0	0
			8	6	2		
56	2A	1	Total	C	O	0	0
			8	6	2		
56	2B	1	Total	C	O	0	0
			8	6	2		

- Molecule 57 is ARGinine (three-letter code: ARG) (formula: $C_6H_{15}N_4O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
57	1B	1	Total	C	N	O	0	0
			12	6	4	2		
57	1F	1	Total	C	N	O	0	0
			12	6	4	2		

- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

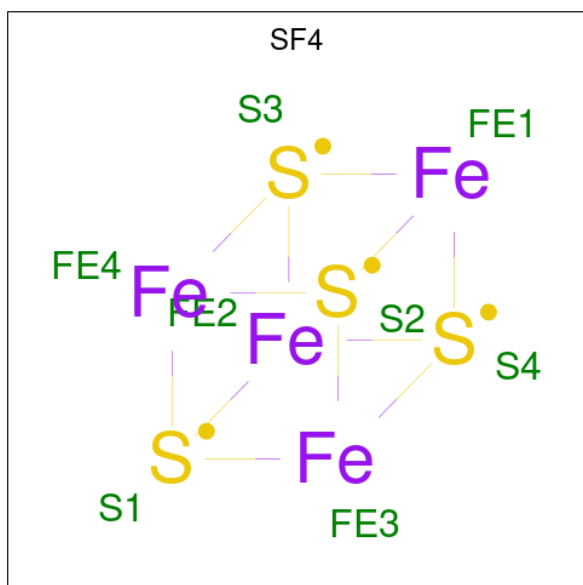
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1Y	1	Total	Zn	0	0
			1	1		
58	14	1	Total	Zn	0	0
			1	1		
58	15	1	Total	Zn	0	0
			1	1		
58	16	1	Total	Zn	0	0
			1	1		
58	19	1	Total	Zn	0	0
			1	1		
58	1n	1	Total	Zn	0	0
			1	1		
58	2Y	1	Total	Zn	0	0
			1	1		
58	24	1	Total	Zn	0	0
			1	1		
58	25	1	Total	Zn	0	0
			1	1		
58	26	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	29	1	Total	Zn	0	0
			1	1		
58	2n	1	Total	Zn	0	0
			1	1		

- Molecule 59 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
59	1d	1	Total	Fe	S	0	0
			8	4	4		
59	2d	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 60 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1A	4016	Total	O	0	0
			4016	4016		
60	1B	110	Total	O	0	0
			110	110		
60	1D	117	Total	O	0	0
			117	117		
60	1E	85	Total	O	0	0
			85	85		
60	1F	70	Total	O	0	0
			70	70		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1G	17	Total	O	0	0
			17	17		
60	1H	14	Total	O	0	0
			14	14		
60	1I	9	Total	O	0	0
			9	9		
60	1N	54	Total	O	0	0
			54	54		
60	1O	21	Total	O	0	0
			21	21		
60	1P	70	Total	O	0	0
			70	70		
60	1Q	40	Total	O	0	0
			40	40		
60	1R	34	Total	O	0	0
			34	34		
60	1S	10	Total	O	0	0
			10	10		
60	1T	36	Total	O	0	0
			36	36		
60	1U	47	Total	O	0	0
			47	47		
60	1V	39	Total	O	0	0
			39	39		
60	1W	23	Total	O	0	0
			23	23		
60	1X	23	Total	O	0	0
			23	23		
60	1Y	17	Total	O	0	0
			17	17		
60	1Z	18	Total	O	0	0
			18	18		
60	10	29	Total	O	0	0
			29	29		
60	11	24	Total	O	0	0
			24	24		
60	12	17	Total	O	0	0
			17	17		
60	13	27	Total	O	0	0
			27	27		
60	14	4	Total	O	0	0
			4	4		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	15	27	Total 27	O 27	0	0
60	16	18	Total 18	O 18	0	0
60	17	18	Total 18	O 18	0	0
60	18	29	Total 29	O 29	0	0
60	19	8	Total 8	O 8	0	0
60	1a	579	Total 579	O 579	0	0
60	1b	1	Total 1	O 1	0	0
60	1c	1	Total 1	O 1	0	0
60	1d	9	Total 9	O 9	0	0
60	1e	5	Total 5	O 5	0	0
60	1f	1	Total 1	O 1	0	0
60	1h	2	Total 2	O 2	0	0
60	1j	1	Total 1	O 1	0	0
60	1k	1	Total 1	O 1	0	0
60	1l	7	Total 7	O 7	0	0
60	1m	1	Total 1	O 1	0	0
60	1o	5	Total 5	O 5	0	0
60	1p	5	Total 5	O 5	0	0
60	1t	1	Total 1	O 1	0	0
60	1u	1	Total 1	O 1	0	0
60	1y	5	Total 5	O 5	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2A	2486	Total 2486	O 2486	0	0
60	2B	64	Total 64	O 64	0	0
60	2D	49	Total 49	O 49	0	0
60	2E	33	Total 33	O 33	0	0
60	2F	19	Total 19	O 19	0	0
60	2G	7	Total 7	O 7	0	0
60	2H	3	Total 3	O 3	0	0
60	2I	4	Total 4	O 4	0	0
60	2N	4	Total 4	O 4	0	0
60	2O	20	Total 20	O 20	0	0
60	2P	29	Total 29	O 29	0	0
60	2Q	29	Total 29	O 29	0	0
60	2R	19	Total 19	O 19	0	0
60	2S	5	Total 5	O 5	0	0
60	2T	12	Total 12	O 12	0	0
60	2U	12	Total 12	O 12	0	0
60	2V	9	Total 9	O 9	0	0
60	2W	16	Total 16	O 16	0	0
60	2X	8	Total 8	O 8	0	0
60	2Y	3	Total 3	O 3	0	0
60	2Z	10	Total 10	O 10	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	20	13	Total 13	O 13	0	0
60	21	23	Total 23	O 23	0	0
60	22	3	Total 3	O 3	0	0
60	23	4	Total 4	O 4	0	0
60	24	2	Total 2	O 2	0	0
60	25	7	Total 7	O 7	0	0
60	26	5	Total 5	O 5	0	0
60	27	11	Total 11	O 11	0	0
60	28	11	Total 11	O 11	0	0
60	29	1	Total 1	O 1	0	0
60	2a	420	Total 420	O 420	0	0
60	2d	8	Total 8	O 8	0	0
60	2e	1	Total 1	O 1	0	0
60	2f	3	Total 3	O 3	0	0
60	2j	1	Total 1	O 1	0	0
60	2l	1	Total 1	O 1	0	0
60	2m	1	Total 1	O 1	0	0
60	2o	4	Total 4	O 4	0	0
60	2p	3	Total 3	O 3	0	0
60	2q	1	Total 1	O 1	0	0
60	2r	3	Total 3	O 3	0	0

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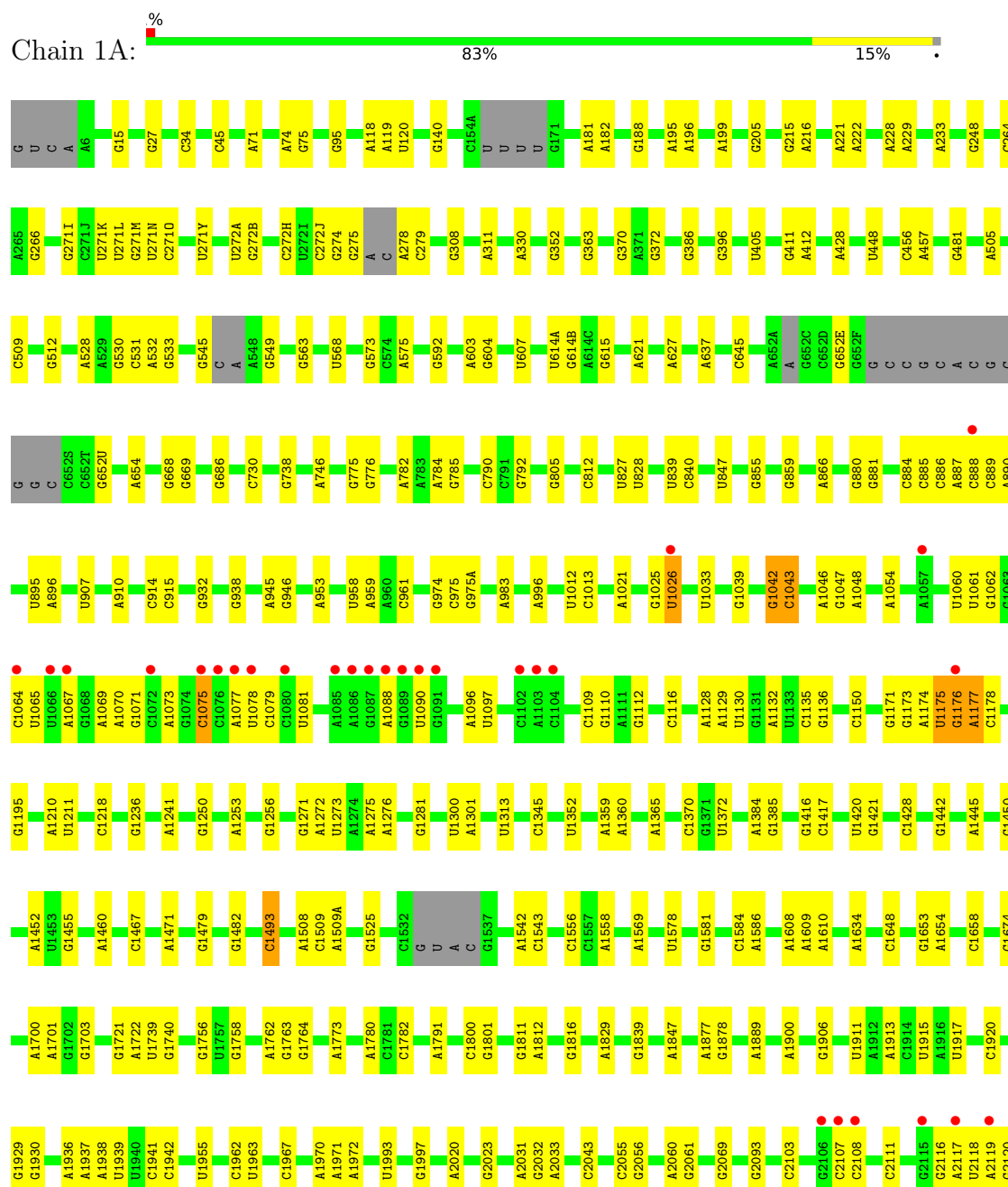
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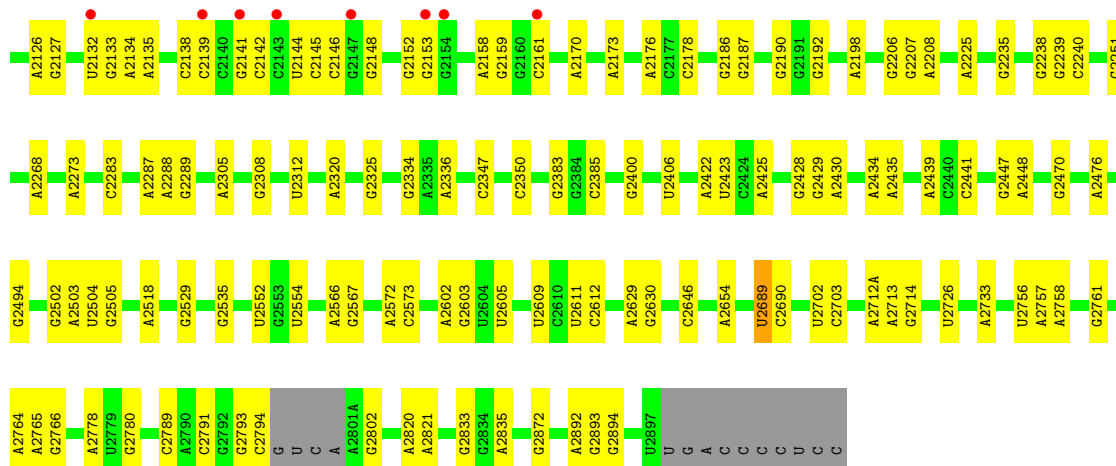
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2t	2	Total	O	0	0
			2	2		
60	2y	3	Total	O	0	0
			3	3		

3 Residue-property plots

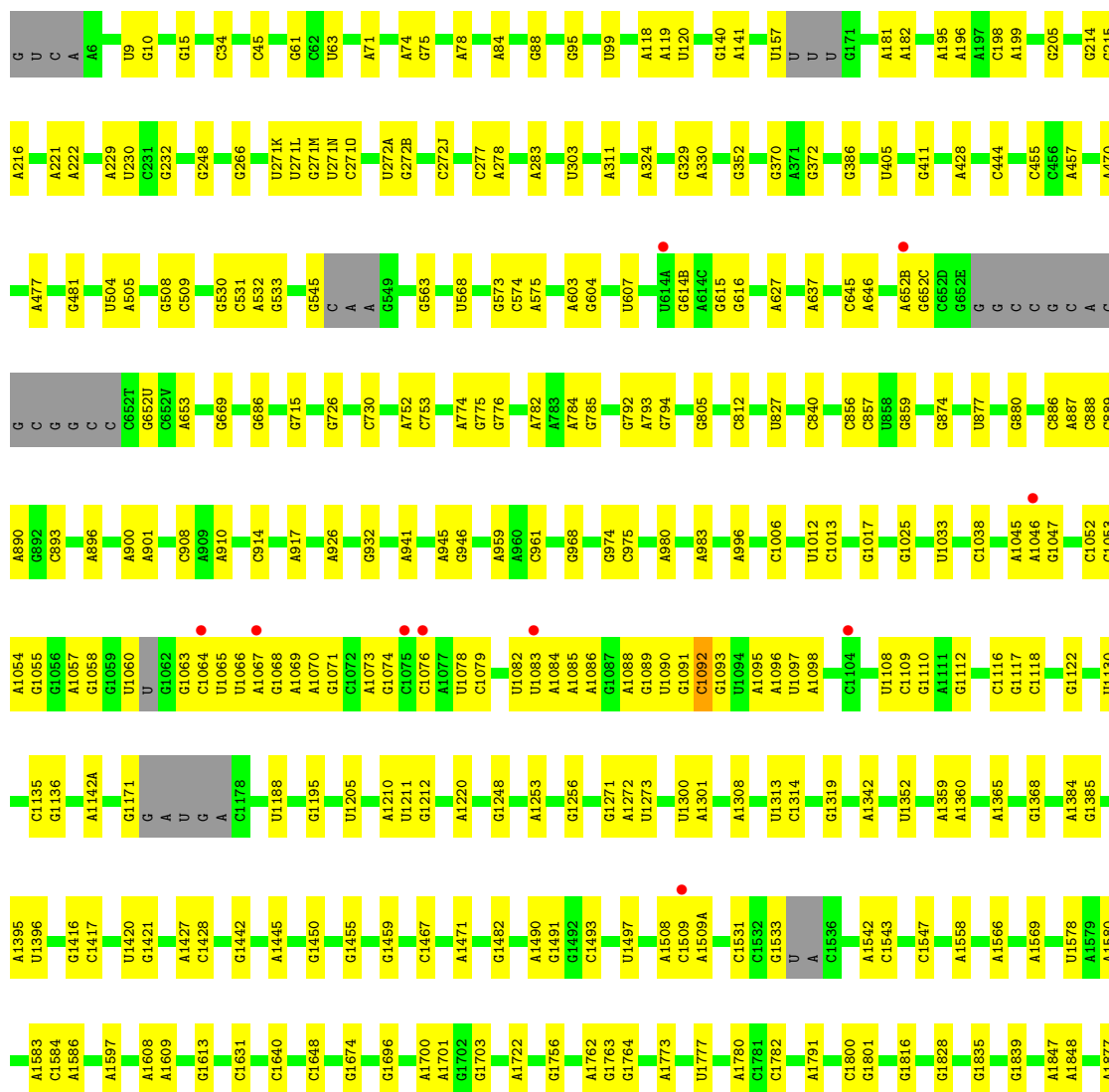
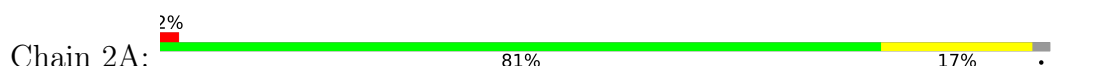
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

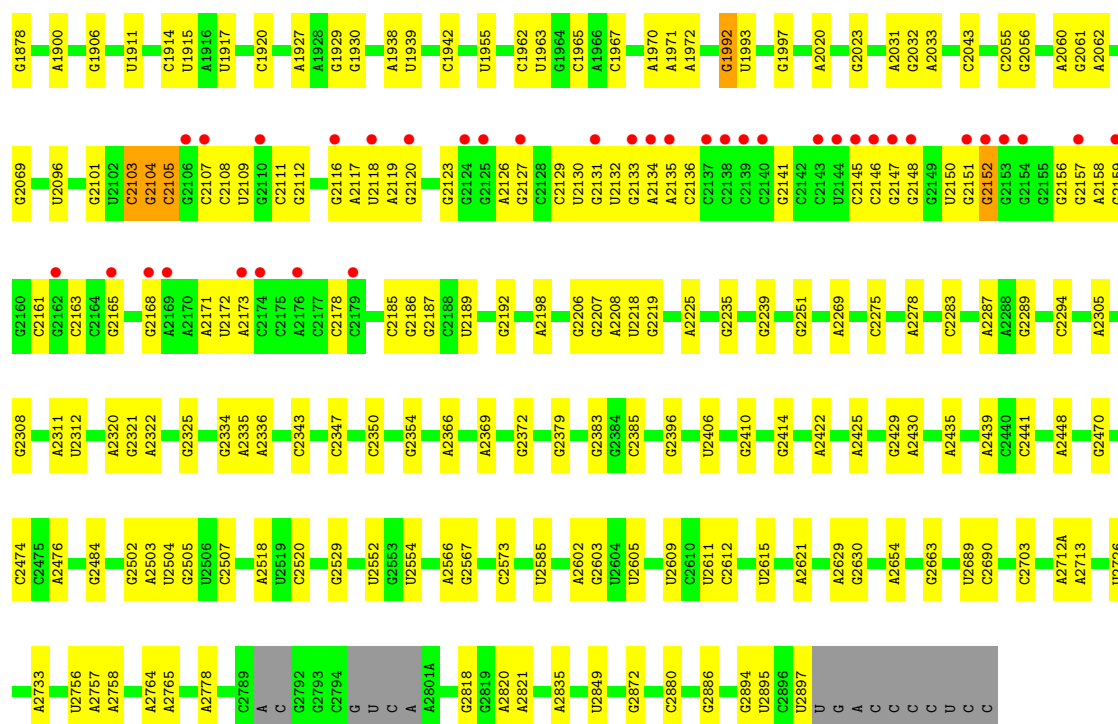
• Molecule 1: 23S Ribosomal RNA





• Molecule 1: 23S Ribosomal RNA





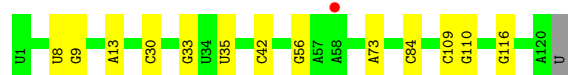
● Molecule 2: 5S Ribosomal RNA

Chain 1B: 91% 8%



● Molecule 2: 5S Ribosomal RNA

Chain 2B: 88% 11%



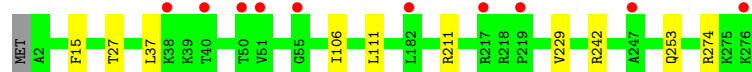
● Molecule 3: 50S ribosomal protein L2

Chain 1D: 93% 6%



● Molecule 3: 50S ribosomal protein L2

Chain 2D: 4% 96%

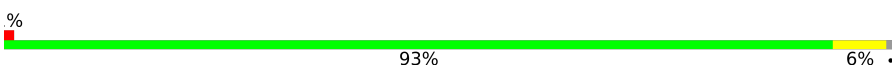


- Molecule 4: 50S ribosomal protein L3

Chain 1E:  94% 5% .




- Molecule 4: 50S ribosomal protein L3

Chain 2E:  93% 6% .



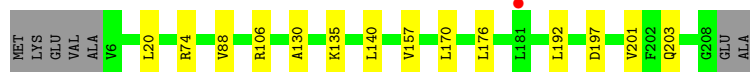
- Molecule 5: 50S ribosomal protein L4

Chain 1F:  89% 8% .



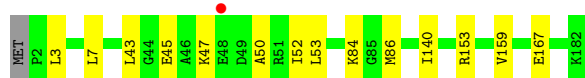
- Molecule 5: 50S ribosomal protein L4

Chain 2F:  90% 7% .



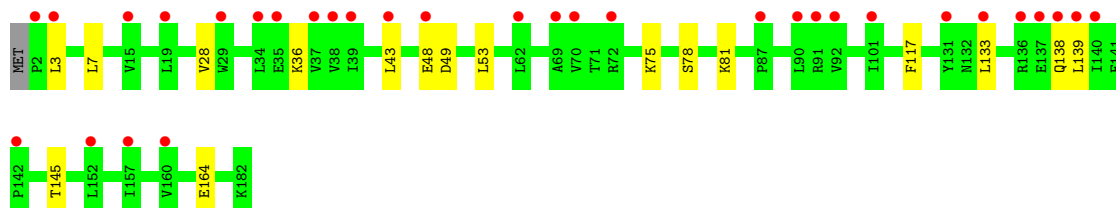
- Molecule 6: 50S ribosomal protein L5

Chain 1G:  92% 8% .



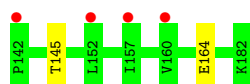
- Molecule 6: 50S ribosomal protein L5

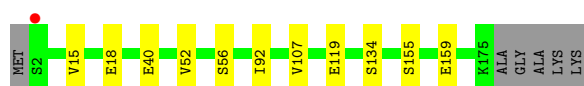
Chain 2G:  18% 90% 9% .



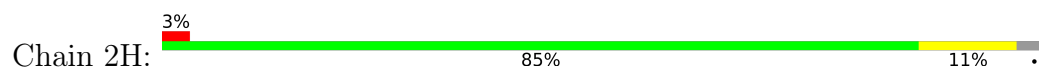
- Molecule 7: 50S ribosomal protein L6

Chain 1H:  91% 6% .

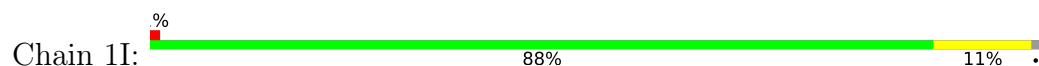




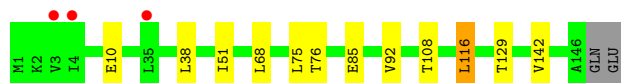
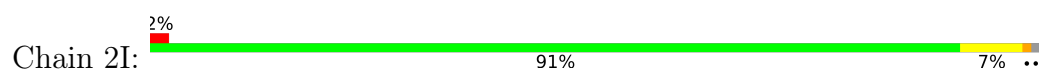
- Molecule 7: 50S ribosomal protein L6



- 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

Chain 2O:  96% .



- Molecule 11: 50S ribosomal protein L15

Chain 1P:  95% . .



- Molecule 11: 50S ribosomal protein L15

Chain 2P:  95% 5% .



- Molecule 12: 50S ribosomal protein L16

Chain 1Q:  94% 6% .



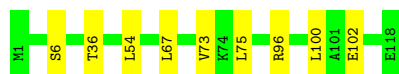
- Molecule 12: 50S ribosomal protein L16

Chain 2Q:  94% 6% .



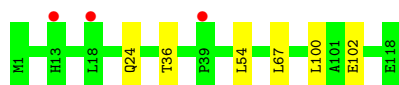
- Molecule 13: 50S ribosomal protein L17

Chain 1R:  92% 8% .



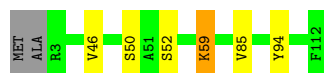
- Molecule 13: 50S ribosomal protein L17

Chain 2R:  95% 5% .




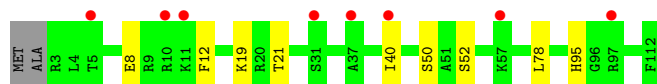
- Molecule 14: 50S ribosomal protein L18

Chain 1S:  93% . .




- Molecule 14: 50S ribosomal protein L18

Chain 2S:  90% 8% .




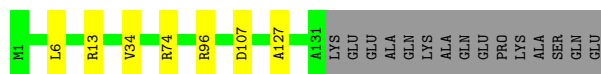
- Molecule 15: 50S ribosomal protein L19

Chain 1T:  86% . 10%



- Molecule 15: 50S ribosomal protein L19

Chain 2T:  85% 5% 10%



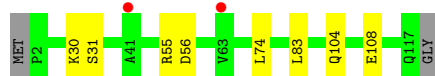
- Molecule 16: 50S ribosomal protein L20

Chain 1U:  91% 8% .



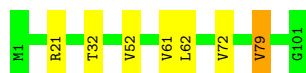
- Molecule 16: 50S ribosomal protein L20

Chain 2U:  92% 7% .



- Molecule 17: 50S ribosomal protein L21

Chain 1V:  93% 6% .



- Molecule 17: 50S ribosomal protein L21

Chain 2V:  92% 8%



- Molecule 18: 50S ribosomal protein L22

Chain 1W:  96% ..



- Molecule 18: 50S ribosomal protein L22

Chain 2W:  95% ..



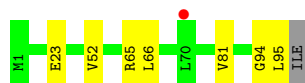
- Molecule 19: 50S ribosomal protein L23

Chain 1X:  90% 9% .



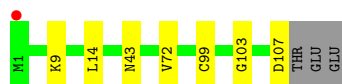
- Molecule 19: 50S ribosomal protein L23

Chain 2X:  92% 7% .



- Molecule 20: 50S ribosomal protein L24

Chain 1Y:  91% 6% .



- Molecule 20: 50S ribosomal protein L24

Chain 2Y:  90% 7% .




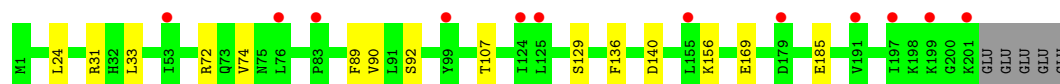
- Molecule 21: 50S ribosomal protein L25

Chain 1Z:  94% 5% •




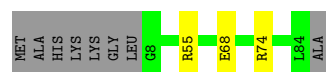
- Molecule 21: 50S ribosomal protein L25

Chain 2Z:  6% 90% 7% •




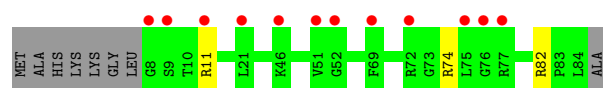
- Molecule 22: 50S ribosomal protein L27

Chain 10:  87% 9% •



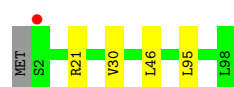
- Molecule 22: 50S ribosomal protein L27

Chain 20:  14% 87% 9% •



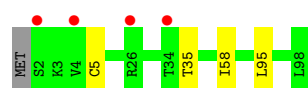
- Molecule 23: 50S ribosomal protein L28

Chain 11:  % 95% • •



- Molecule 23: 50S ribosomal protein L28

Chain 21:  4% 95% • •



- Molecule 24: 50S ribosomal protein L29

Chain 12:  90% 7% •




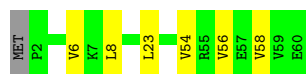
- Molecule 24: 50S ribosomal protein L29

Chain 22:  92% 6% .




- Molecule 25: 50S ribosomal protein L30

Chain 13:  88% 10% .




- Molecule 25: 50S ribosomal protein L30

Chain 23:  88% 10% .




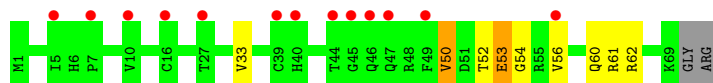
- Molecule 26: 50S ribosomal protein L31

Chain 14:  80% 17% .



- Molecule 26: 50S ribosomal protein L31

Chain 24:  18% 85% 10% . .



- Molecule 27: 50S ribosomal protein L32

Chain 15:  93% 5% .




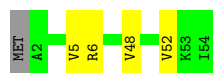
- Molecule 27: 50S ribosomal protein L32

Chain 25:  2% 93% 5% .




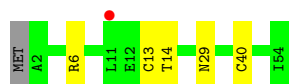
- Molecule 28: 50S ribosomal protein L33

Chain 16:  91% 7% .



• Molecule 28: 50S ribosomal protein L33

Chain 26:  89% 9% .



• Molecule 29: 50S ribosomal protein L34

Chain 17:  98% .



• Molecule 29: 50S ribosomal protein L34

Chain 27:  98% .

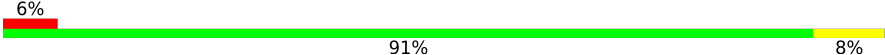


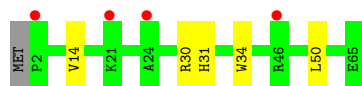
• Molecule 30: 50S ribosomal protein L35

Chain 18:  94% 5% .



• Molecule 30: 50S ribosomal protein L35

Chain 28:  91% 8% .



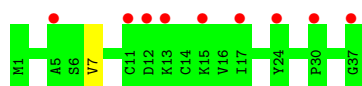
• Molecule 31: 50S ribosomal protein L36

Chain 19:  100%

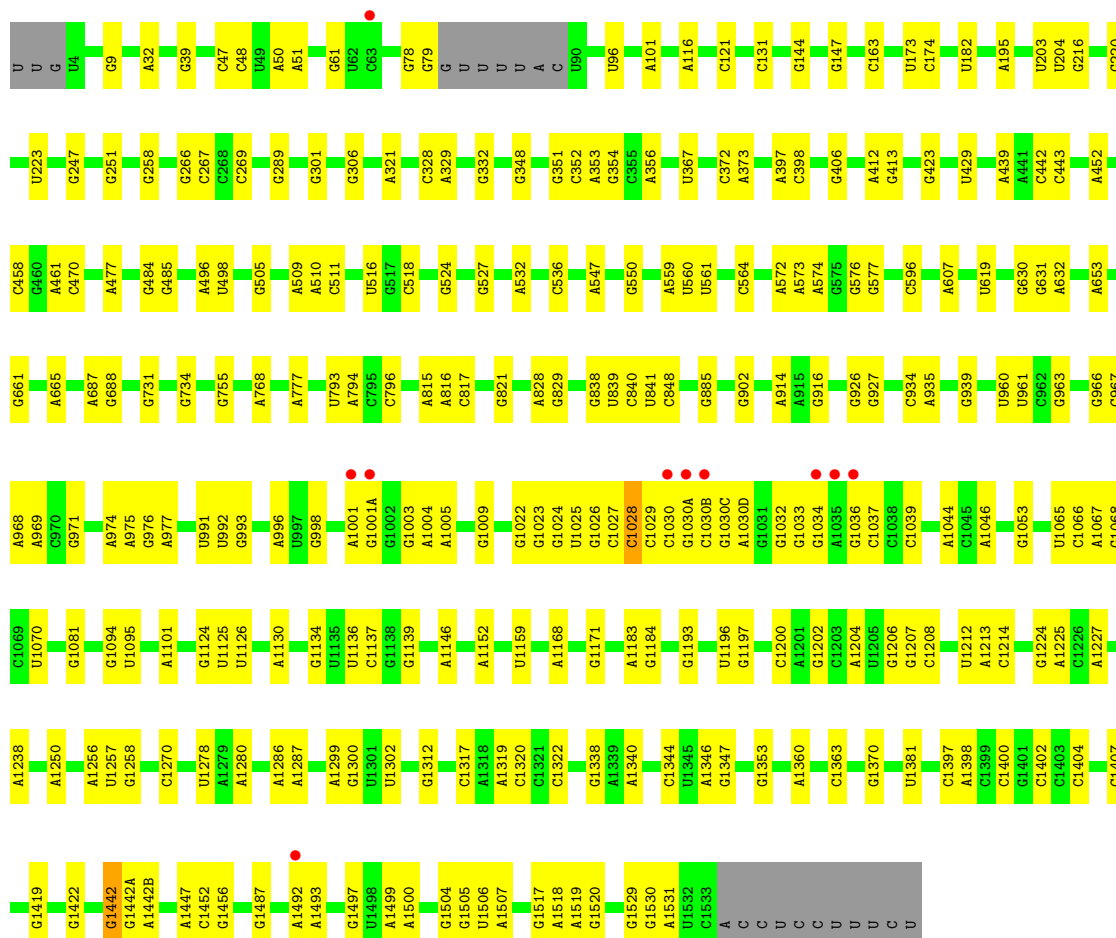
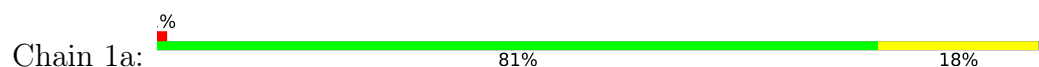
There are no outlier residues recorded for this chain.

• Molecule 31: 50S ribosomal protein L36

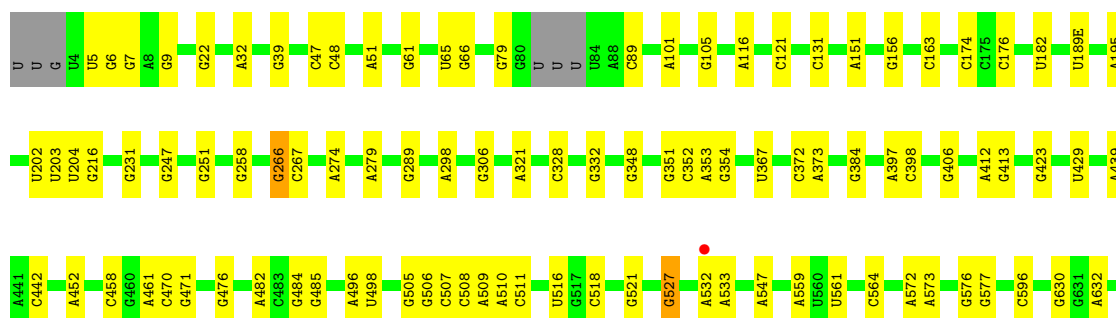
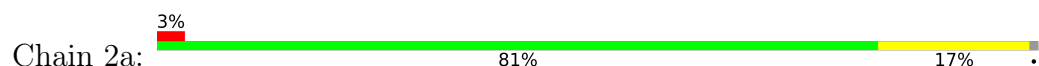
Chain 29:  97% .

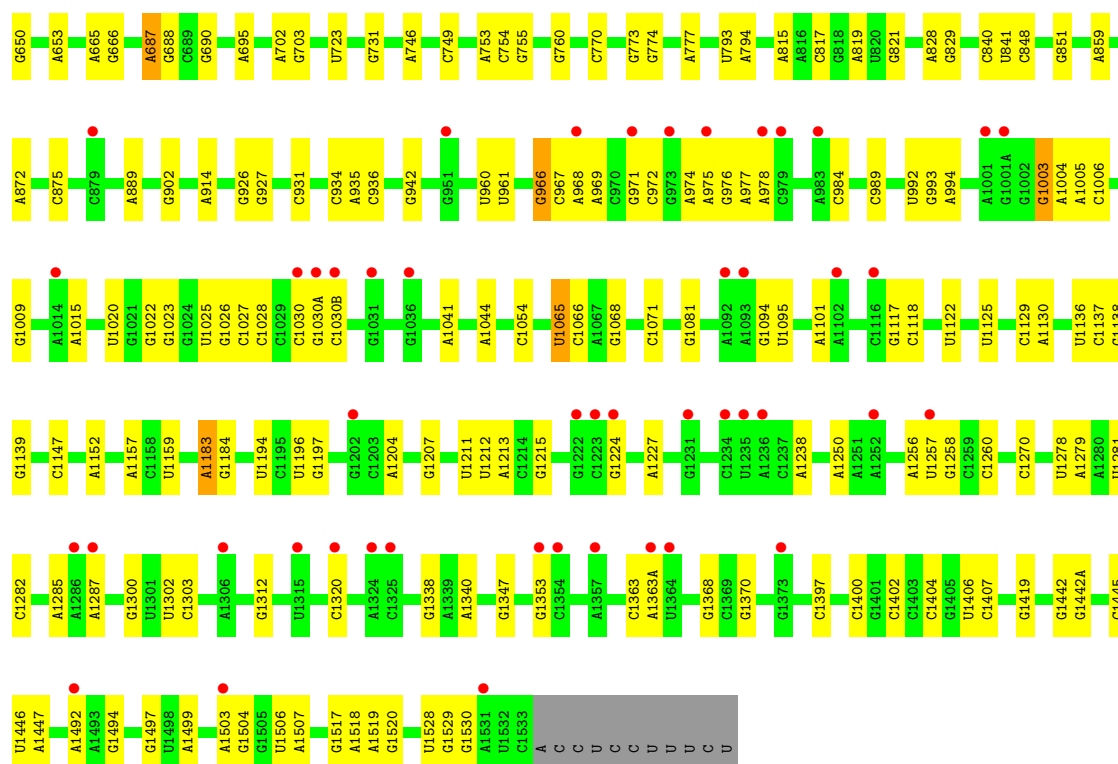


• Molecule 32: 16S Ribosomal RNA

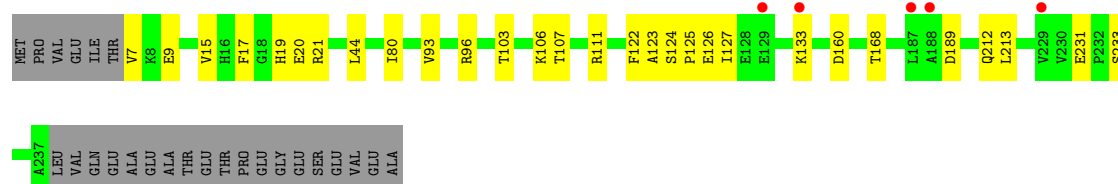
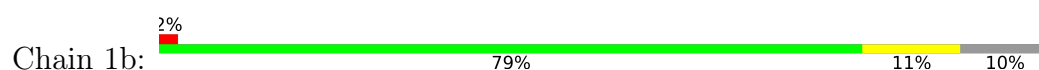


• Molecule 32: 16S Ribosomal RNA

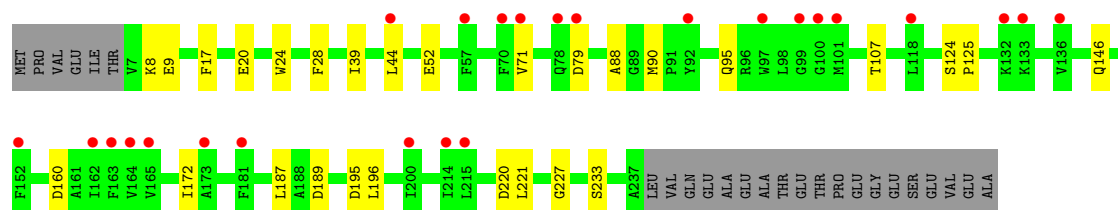
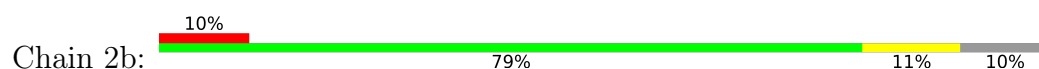




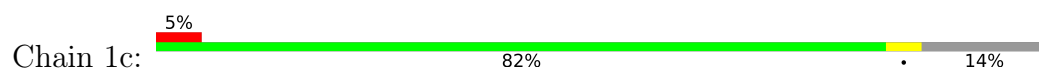
• Molecule 33: 30S ribosomal protein S2

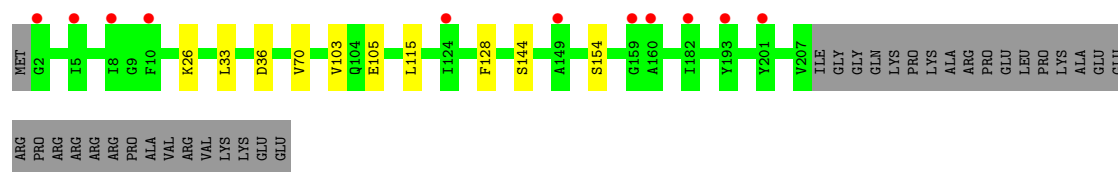


• Molecule 33: 30S ribosomal protein S2

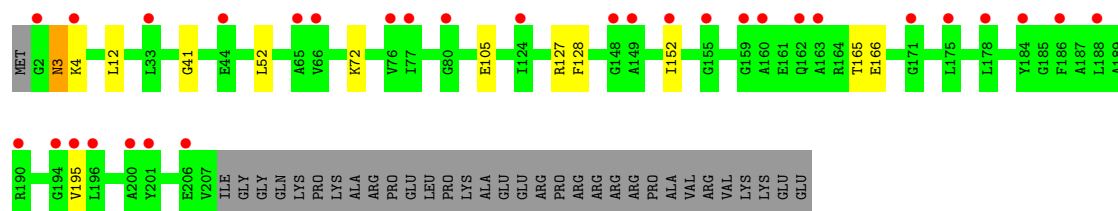
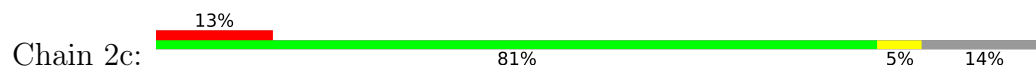


• Molecule 34: 30S ribosomal protein S3

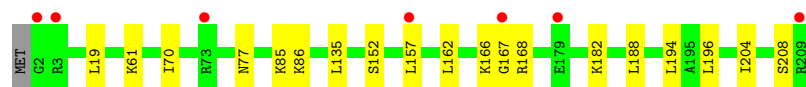




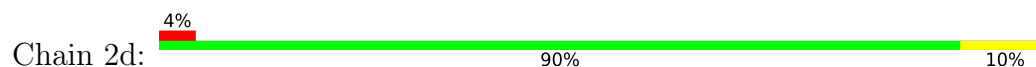
- Molecule 34: 30S ribosomal protein S3



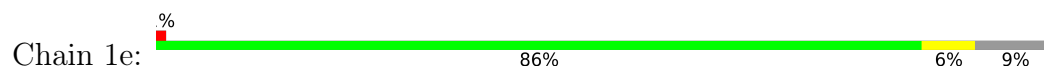
- Molecule 35: 30S ribosomal protein S4



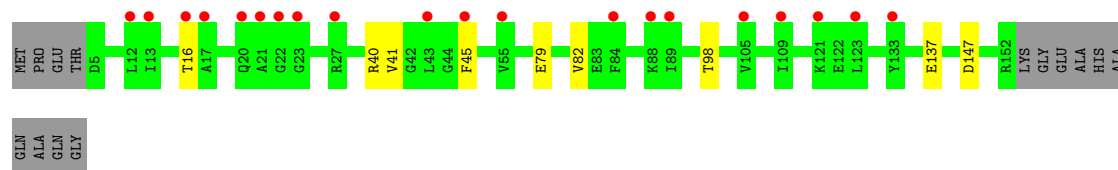
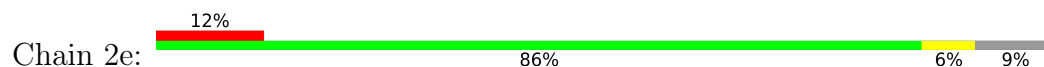
- Molecule 35: 30S ribosomal protein S4




- Molecule 36: 30S ribosomal protein S5



- Molecule 36: 30S ribosomal protein S5

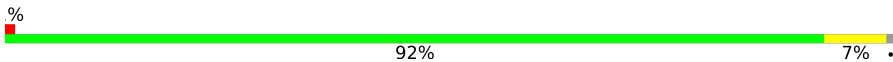


- Molecule 37: 30S ribosomal protein S6

Chain 1f:  90% 9% .



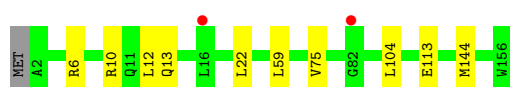
- Molecule 37: 30S ribosomal protein S6

Chain 2f:  92% 7% .



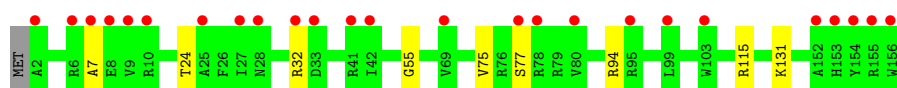
- Molecule 38: 30S ribosomal protein S7

Chain 1g:  93% 6% .



- Molecule 38: 30S ribosomal protein S7

Chain 2g:  16% 94% 6% .



- Molecule 39: 30S ribosomal protein S8

Chain 1h:  91% 7% ..

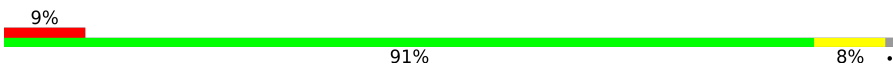


- Molecule 39: 30S ribosomal protein S8

Chain 2h:  3% 93% 7% .

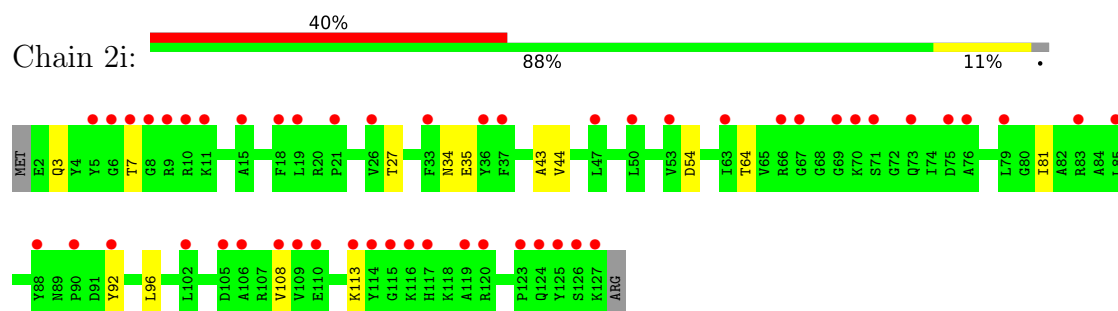


- Molecule 40: 30S ribosomal protein S9

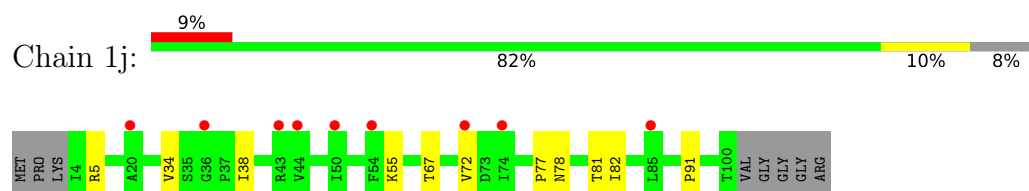
Chain 1i:  9% 91% 8% .



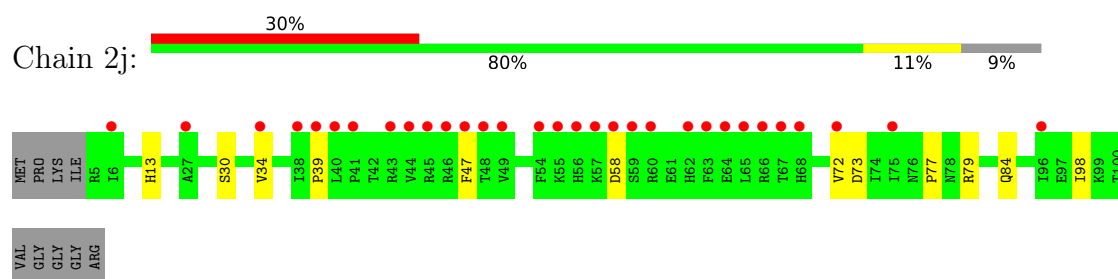
- Molecule 40: 30S ribosomal protein S9



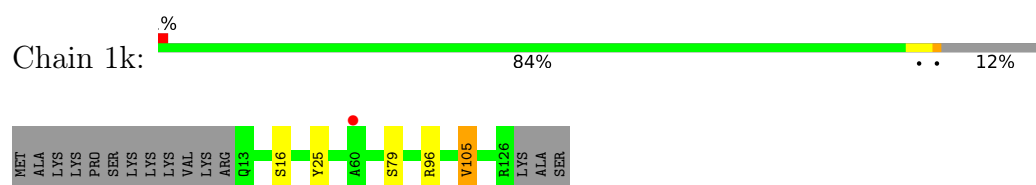
- Molecule 41: 30S ribosomal protein S10



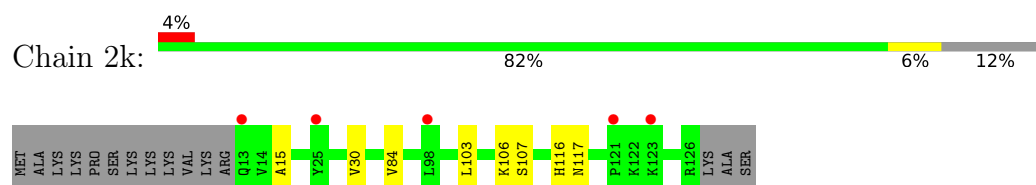
- Molecule 41: 30S ribosomal protein S10



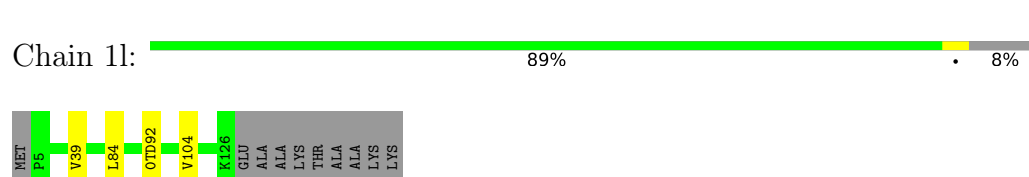
- Molecule 42: 30S ribosomal protein S11



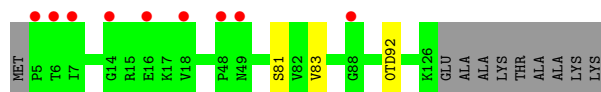
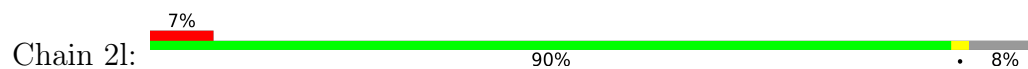
- Molecule 42: 30S ribosomal protein S11



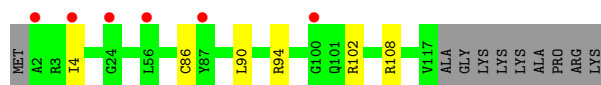
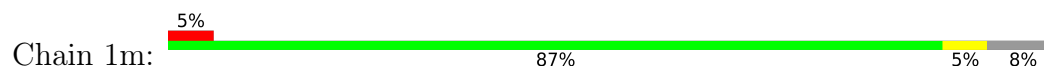
- Molecule 43: 30S ribosomal protein S12



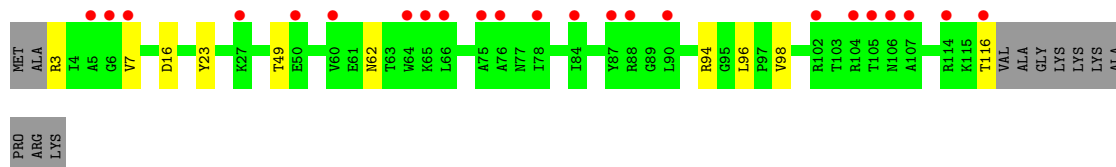
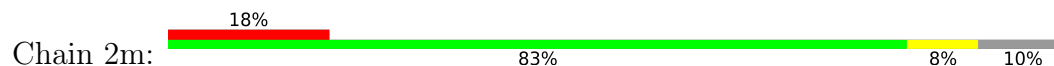
- Molecule 43: 30S ribosomal protein S12



- Molecule 44: 30S ribosomal protein S13



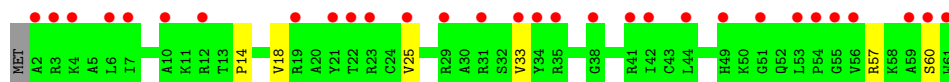
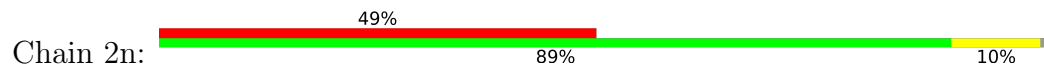
- Molecule 44: 30S ribosomal protein S13



- Molecule 45: 30S ribosomal protein S14 type Z



- Molecule 45: 30S ribosomal protein S14 type Z

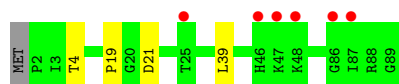


- Molecule 46: 30S ribosomal protein S15

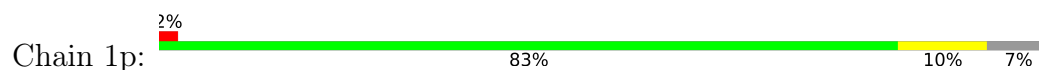


- Molecule 46: 30S ribosomal protein S15

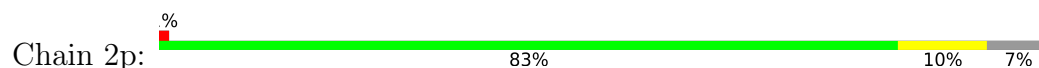




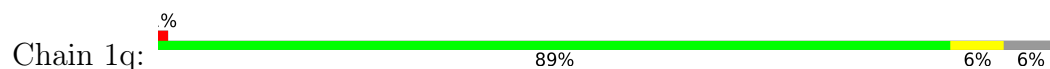
- Molecule 47: 30S ribosomal protein S16



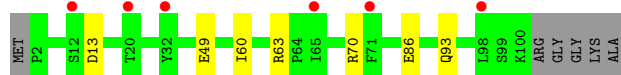
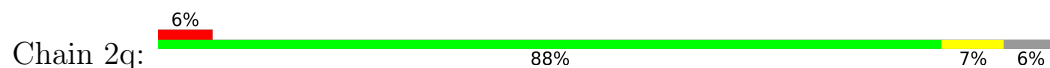
- Molecule 47: 30S ribosomal protein S16



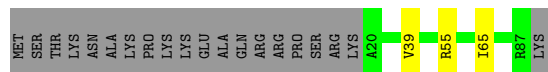
- Molecule 48: 30S ribosomal protein S17



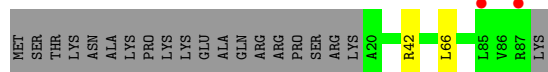
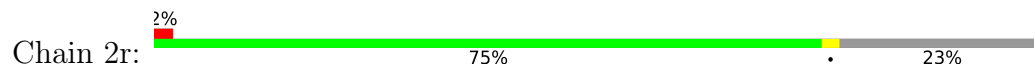
- Molecule 48: 30S ribosomal protein S17



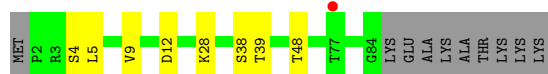
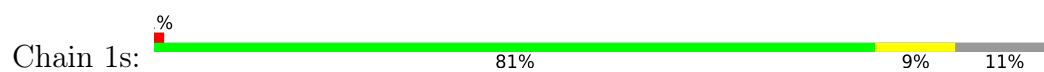
- Molecule 49: 30S ribosomal protein S18



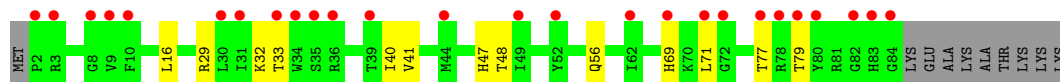
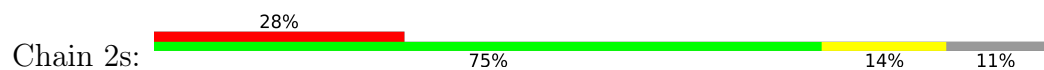
- Molecule 49: 30S ribosomal protein S18



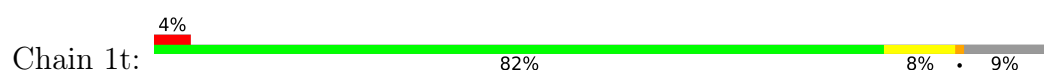
- Molecule 50: 30S ribosomal protein S19



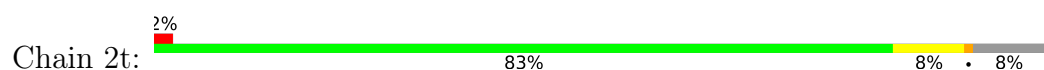
- Molecule 50: 30S ribosomal protein S19



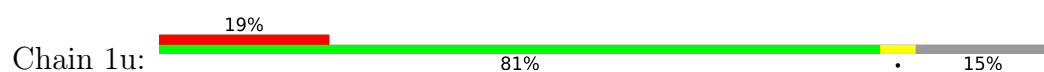
- Molecule 51: 30S ribosomal protein S20



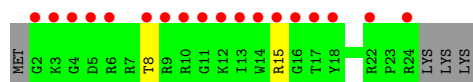
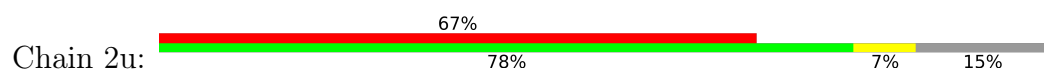
- Molecule 51: 30S ribosomal protein S20



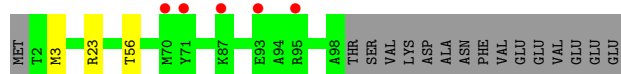
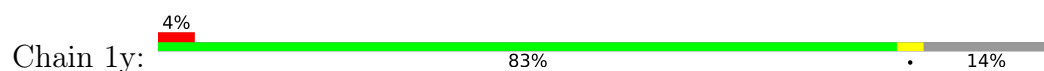
- Molecule 52: 30S ribosomal protein Thx



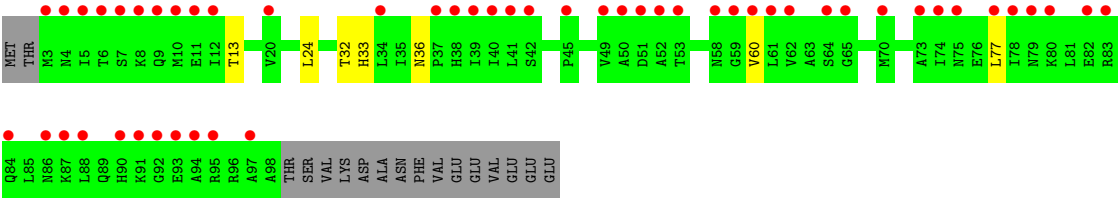
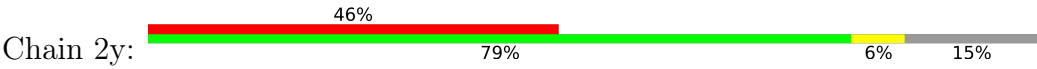
- Molecule 52: 30S ribosomal protein Thx



- Molecule 53: Ribosome-associated inhibitor A



● Molecule 53: Ribosome-associated inhibitor A



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.50Å 448.64Å 621.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	152.16 – 2.80 255.39 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.4 (152.16-2.80) 97.4 (255.39-2.80)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 2.82Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.218 , 0.268 0.218 , 0.268	Depositor DCC
R_{free} test set	69237 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	51.8	Xtriage
Anisotropy	0.248	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 60.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	298171	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.78% 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: OMG, 7MG, 5MU, MA6, 0TD, PSU, 4OC, 2MU, MG, MPD, YXM, 2MA, 5MC, UR3, ZN, 2MG, SF4, M2G

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	0.33	0/69029	0.81	20/107746 (0.0%)
1	2A	0.28	1/68901 (0.0%)	0.79	28/107544 (0.0%)
2	1B	0.29	0/2876	0.77	0/4486
2	2B	0.24	0/2878	0.77	0/4490
3	1D	0.29	0/2181	0.50	0/2940
3	2D	0.28	0/2186	0.48	0/2944
4	1E	0.27	0/1592	0.48	0/2149
4	2E	0.27	0/1592	0.48	0/2149
5	1F	0.28	0/1619	0.46	0/2193
5	2F	0.27	0/1615	0.46	0/2188
6	1G	0.26	0/1451	0.45	0/1961
6	2G	0.26	0/1449	0.44	0/1957
7	1H	0.27	0/1356	0.45	0/1834
7	2H	0.26	0/1350	0.45	0/1826
8	1I	0.25	0/1109	0.46	0/1512
8	2I	0.24	0/1091	0.44	0/1490
9	1N	0.28	0/1148	0.44	0/1547
9	2N	0.25	0/1144	0.42	0/1543
10	1O	0.31	0/943	0.51	0/1269
10	2O	0.28	0/943	0.50	0/1269
11	1P	0.28	0/1152	0.49	0/1533
11	2P	0.26	0/1152	0.47	0/1533
12	1Q	0.27	0/1143	0.46	0/1527
12	2Q	0.27	0/1143	0.44	0/1527
13	1R	0.25	0/982	0.47	0/1312
13	2R	0.25	0/982	0.44	0/1312
14	1S	0.26	0/887	0.46	0/1180
14	2S	0.25	0/880	0.47	0/1172
15	1T	0.28	0/1105	0.46	0/1477
15	2T	0.26	0/1097	0.42	0/1468
16	1U	0.27	0/977	0.44	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.25	0/977	0.39	0/1301
17	1V	0.27	0/786	0.49	0/1053
17	2V	0.27	0/782	0.49	0/1049
18	1W	0.27	0/897	0.45	0/1205
18	2W	0.26	0/897	0.43	0/1205
19	1X	0.29	0/764	0.49	0/1025
19	2X	0.27	0/764	0.48	0/1025
20	1Y	0.28	0/823	0.49	0/1099
20	2Y	0.26	0/823	0.47	0/1100
21	1Z	0.27	0/1620	0.46	0/2200
21	2Z	0.26	0/1590	0.46	0/2162
22	10	0.29	0/616	0.50	0/821
22	20	0.26	0/616	0.47	0/821
23	11	0.27	0/761	0.46	0/1013
23	21	0.27	0/766	0.48	0/1018
24	12	0.25	0/590	0.43	0/781
24	22	0.24	0/594	0.38	0/785
25	13	0.26	0/474	0.45	0/635
25	23	0.25	0/469	0.41	0/630
26	14	0.26	0/559	0.49	0/754
26	24	0.29	0/549	0.51	0/741
27	15	0.27	0/473	0.48	0/639
27	25	0.26	0/469	0.43	0/635
28	16	0.26	0/460	0.49	0/613
28	26	0.25	0/456	0.45	0/608
29	17	0.26	0/426	0.45	0/561
29	27	0.25	0/426	0.45	0/561
30	18	0.28	0/525	0.47	0/691
30	28	0.26	0/525	0.44	0/691
31	19	0.25	0/310	0.44	0/407
31	29	0.25	0/310	0.45	0/407
32	1a	0.26	0/35795	0.79	5/55864 (0.0%)
32	2a	0.25	0/35890	0.80	16/56012 (0.0%)
33	1b	0.26	0/1876	0.44	0/2533
33	2b	0.27	0/1860	0.46	0/2518
34	1c	0.25	0/1582	0.43	0/2137
34	2c	0.25	0/1566	0.46	0/2119
35	1d	0.26	0/1695	0.44	0/2274
35	2d	0.25	0/1698	0.41	0/2277
36	1e	0.26	0/1149	0.46	0/1548
36	2e	0.26	0/1149	0.46	0/1548
37	1f	0.26	0/827	0.45	0/1120
37	2f	0.25	0/829	0.44	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.26	0/1254	0.39	0/1683
38	2g	0.24	0/1248	0.39	0/1676
39	1h	0.25	0/1118	0.45	0/1506
39	2h	0.26	0/1108	0.44	0/1494
40	1i	0.27	0/1005	0.45	0/1351
40	2i	0.26	0/985	0.43	0/1329
41	1j	0.26	0/732	0.43	0/993
41	2j	0.25	0/723	0.45	0/984
42	1k	0.26	0/849	0.45	0/1150
42	2k	0.25	0/848	0.48	0/1149
43	1l	0.26	0/937	0.48	0/1260
43	2l	0.25	0/937	0.45	0/1260
44	1m	0.25	0/924	0.46	0/1242
44	2m	0.26	0/905	0.45	0/1217
45	1n	0.26	0/501	0.44	0/664
45	2n	0.26	0/501	0.42	0/664
46	1o	0.25	0/739	0.40	0/985
46	2o	0.24	0/739	0.39	0/985
47	1p	0.25	0/697	0.48	0/939
47	2p	0.25	0/693	0.45	0/935
48	1q	0.25	0/836	0.45	0/1117
48	2q	0.25	0/836	0.45	0/1117
49	1r	0.26	0/560	0.42	0/746
49	2r	0.26	0/560	0.43	0/746
50	1s	0.24	0/663	0.43	0/895
50	2s	0.25	0/660	0.45	0/893
51	1t	0.25	0/734	0.37	0/969
51	2t	0.25	0/736	0.37	0/976
52	1u	0.25	0/203	0.43	0/266
52	2u	0.24	0/203	0.47	0/266
53	1y	0.24	0/776	0.44	0/1048
53	2y	0.25	0/761	0.45	0/1030
All	All	0.28	1/309937 (0.0%)	0.72	69/463223 (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
21	2Z	0	1
33	1b	0	2
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	2104	G	N1-C2	-5.65	1.33	1.37

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2104	G	C5-C6-O6	12.87	136.32	128.60
1	2A	2104	G	N3-C2-N2	11.92	128.25	119.90
1	1A	1042	G	OP1-P-O3'	-11.63	79.62	105.20
1	2A	2185	C	N1-C2-O2	10.89	125.44	118.90
1	2A	2104	G	N1-C2-N2	-10.54	106.71	116.20
1	2A	2185	C	C2-N3-C4	9.80	124.80	119.90
1	2A	1092	C	C2-N1-C1'	9.18	128.89	118.80
1	2A	1092	C	N1-C2-O2	8.59	124.06	118.90
1	1A	1042	G	OP2-P-O3'	-8.16	87.26	105.20
1	1A	1177	A	O5'-P-OP1	-7.70	98.77	105.70
1	1A	1043	C	OP1-P-OP2	7.52	130.88	119.60
1	2A	2104	G	C6-N1-C2	7.35	129.51	125.10
1	1A	1064	C	N1-C2-O2	7.28	123.27	118.90
1	2A	2104	G	N1-C6-O6	-7.10	115.64	119.90
1	2A	1092	C	N3-C2-O2	-7.02	116.99	121.90
1	2A	2104	G	C5-C6-N1	-6.94	108.03	111.50
32	2a	1003	G	C8-N9-C4	-6.92	103.63	106.40
32	1a	839	U	P-O3'-C3'	6.80	127.86	119.70
1	2A	1092	C	C6-N1-C2	-6.79	117.58	120.30
1	2A	2185	C	C5-C6-N1	6.75	124.38	121.00
32	2a	1003	G	N3-C4-C5	-6.62	125.29	128.60
32	2a	266	G	P-O3'-C3'	6.44	127.43	119.70
32	2a	1183	A	P-O3'-C3'	6.34	127.31	119.70
1	1A	1075	C	C2-N1-C1'	6.18	125.60	118.80
32	1a	839	U	OP1-P-O3'	6.11	118.63	105.20
1	2A	1092	C	C6-N1-C1'	-6.08	113.50	120.80
1	2A	2104	G	C4-N9-C1'	6.04	134.36	126.50
1	2A	1313	U	C2-N1-C1'	6.04	124.95	117.70
1	1A	1493	C	C2-N1-C1'	6.03	125.44	118.80
1	1A	1026	U	N1-C2-O2	6.00	127.00	122.80
1	1A	1176	G	OP1-P-O3'	6.00	118.39	105.20
32	2a	1183	A	OP1-P-O3'	5.95	118.29	105.20
1	1A	512	G	O4'-C1'-N9	5.92	112.94	108.20
32	2a	1003	G	C4-N9-C1'	5.81	134.05	126.50
1	2A	2104	G	C8-N9-C1'	-5.80	119.46	127.00
32	2a	754	C	C2-N1-C1'	5.79	125.17	118.80
1	1A	847	U	C2-N1-C1'	5.72	124.57	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1026	U	N3-C2-O2	-5.69	118.22	122.20
32	2a	1054	C	C2-N1-C1'	5.60	124.96	118.80
1	2A	2103	C	N1-C2-O2	5.59	122.25	118.90
1	2A	2185	C	C5-C4-N4	5.58	124.11	120.20
32	1a	1442	G	P-O3'-C3'	5.55	126.36	119.70
32	2a	1030	C	N1-C2-O2	5.54	122.22	118.90
1	2A	1313	U	N1-C2-O2	5.49	126.65	122.80
32	2a	1003	G	N7-C8-N9	5.47	115.83	113.10
1	2A	2185	C	C4-C5-C6	-5.47	114.67	117.40
1	2A	1097	U	C2-N1-C1'	5.39	124.17	117.70
1	2A	2152	G	C5-C6-O6	5.38	131.82	128.60
1	1A	1372	U	C5-C4-O4	-5.32	122.71	125.90
1	2A	1092	C	C5-C6-N1	5.31	123.65	121.00
1	2A	2185	C	N3-C4-N4	-5.28	114.31	118.00
32	2a	1065	U	P-O3'-C3'	5.26	126.02	119.70
1	1A	1075	C	N1-C2-O2	5.25	122.05	118.90
1	1A	1075	C	C6-N1-C1'	-5.24	114.52	120.80
32	1a	1067	A	P-O3'-C3'	5.22	125.96	119.70
1	1A	1313	U	C2-N1-C1'	5.21	123.95	117.70
1	1A	1026	U	C2-N1-C1'	5.17	123.91	117.70
1	2A	1992	G	P-O3'-C3'	5.16	125.89	119.70
1	1A	1175	U	P-O3'-C3'	5.16	125.89	119.70
32	1a	1028	C	C2-N3-C4	5.15	122.47	119.90
32	2a	754	C	N1-C2-O2	5.11	121.97	118.90
1	1A	271(Y)	U	O4'-C1'-N1	5.10	112.28	108.20
32	2a	65	U	P-O3'-C3'	5.10	125.82	119.70
32	2a	1003	G	C2-N3-C4	5.08	114.44	111.90
1	2A	1313	U	N3-C2-O2	-5.08	118.64	122.20
32	2a	687	A	P-O3'-C3'	5.07	125.78	119.70
1	2A	2105	C	C5-C6-N1	5.05	123.53	121.00
1	1A	2689	U	P-O3'-C3'	5.03	125.73	119.70
32	2a	1054	C	C6-N1-C2	-5.01	118.30	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
33	1b	123	ALA	Peptide
33	1b	124	SER	Peptide
21	2Z	136	PHE	Peptide

5.2 Too-close contacts ⓘ

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	257 (94%)	16 (6%)	0	100	100
3	2D	273/276 (99%)	252 (92%)	21 (8%)	0	100	100
4	1E	202/206 (98%)	192 (95%)	8 (4%)	2 (1%)	15	44
4	2E	202/206 (98%)	187 (93%)	12 (6%)	3 (2%)	10	33
5	1F	201/210 (96%)	196 (98%)	4 (2%)	1 (0%)	29	61
5	2F	201/210 (96%)	194 (96%)	6 (3%)	1 (0%)	29	61
6	1G	179/182 (98%)	157 (88%)	19 (11%)	3 (2%)	9	29
6	2G	179/182 (98%)	155 (87%)	20 (11%)	4 (2%)	6	22
7	1H	172/180 (96%)	166 (96%)	4 (2%)	2 (1%)	13	39
7	2H	171/180 (95%)	149 (87%)	20 (12%)	2 (1%)	13	39
8	1I	145/148 (98%)	124 (86%)	21 (14%)	0	100	100
8	2I	144/148 (97%)	133 (92%)	9 (6%)	2 (1%)	11	34
9	1N	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
9	2N	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
10	1O	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
10	2O	120/122 (98%)	110 (92%)	10 (8%)	0	100	100
11	1P	147/150 (98%)	141 (96%)	6 (4%)	0	100	100
11	2P	147/150 (98%)	135 (92%)	10 (7%)	2 (1%)	11	34
12	1Q	139/141 (99%)	130 (94%)	8 (6%)	1 (1%)	22	53
12	2Q	139/141 (99%)	131 (94%)	7 (5%)	1 (1%)	22	53
13	1R	116/118 (98%)	110 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	2R	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
14	1S	108/112 (96%)	101 (94%)	5 (5%)	2 (2%)	8	26
14	2S	108/112 (96%)	101 (94%)	7 (6%)	0	100	100
15	1T	129/146 (88%)	120 (93%)	9 (7%)	0	100	100
15	2T	129/146 (88%)	118 (92%)	10 (8%)	1 (1%)	19	49
16	1U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
16	2U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
17	1V	99/101 (98%)	92 (93%)	6 (6%)	1 (1%)	15	44
17	2V	99/101 (98%)	89 (90%)	10 (10%)	0	100	100
18	1W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
18	2W	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
19	1X	93/96 (97%)	88 (95%)	3 (3%)	2 (2%)	6	22
19	2X	93/96 (97%)	86 (92%)	6 (6%)	1 (1%)	14	41
20	1Y	105/110 (96%)	93 (89%)	11 (10%)	1 (1%)	15	44
20	2Y	105/110 (96%)	98 (93%)	7 (7%)	0	100	100
21	1Z	201/206 (98%)	188 (94%)	13 (6%)	0	100	100
21	2Z	199/206 (97%)	175 (88%)	21 (11%)	3 (2%)	10	33
22	10	75/85 (88%)	72 (96%)	3 (4%)	0	100	100
22	20	75/85 (88%)	72 (96%)	3 (4%)	0	100	100
23	11	95/98 (97%)	94 (99%)	1 (1%)	0	100	100
23	21	95/98 (97%)	91 (96%)	4 (4%)	0	100	100
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
25	13	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
25	23	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
26	14	67/71 (94%)	51 (76%)	12 (18%)	4 (6%)	1	4
26	24	67/71 (94%)	45 (67%)	18 (27%)	4 (6%)	1	4
27	15	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	25	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
28	16	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
28	26	51/54 (94%)	49 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	17	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
29	27	46/49 (94%)	46 (100%)	0	0	100	100
30	18	62/65 (95%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
31	19	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
31	29	35/37 (95%)	35 (100%)	0	0	100	100
33	1b	229/256 (90%)	202 (88%)	19 (8%)	8 (4%)	3	12
33	2b	229/256 (90%)	191 (83%)	31 (14%)	7 (3%)	4	14
34	1c	204/239 (85%)	188 (92%)	16 (8%)	0	100	100
34	2c	204/239 (85%)	170 (83%)	30 (15%)	4 (2%)	7	24
35	1d	206/209 (99%)	191 (93%)	14 (7%)	1 (0%)	29	61
35	2d	206/209 (99%)	183 (89%)	22 (11%)	1 (0%)	29	61
36	1e	146/162 (90%)	140 (96%)	4 (3%)	2 (1%)	11	34
36	2e	146/162 (90%)	136 (93%)	9 (6%)	1 (1%)	22	53
37	1f	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
37	2f	98/101 (97%)	93 (95%)	4 (4%)	1 (1%)	15	44
38	1g	153/156 (98%)	144 (94%)	9 (6%)	0	100	100
38	2g	153/156 (98%)	136 (89%)	13 (8%)	4 (3%)	5	18
39	1h	135/138 (98%)	126 (93%)	7 (5%)	2 (2%)	10	33
39	2h	135/138 (98%)	125 (93%)	10 (7%)	0	100	100
40	1i	125/128 (98%)	111 (89%)	14 (11%)	0	100	100
40	2i	124/128 (97%)	107 (86%)	13 (10%)	4 (3%)	4	13
41	1j	95/105 (90%)	81 (85%)	9 (10%)	5 (5%)	2	6
41	2j	94/105 (90%)	81 (86%)	10 (11%)	3 (3%)	4	13
42	1k	112/129 (87%)	97 (87%)	14 (12%)	1 (1%)	17	46
42	2k	112/129 (87%)	99 (88%)	11 (10%)	2 (2%)	8	28
43	1l	119/132 (90%)	111 (93%)	8 (7%)	0	100	100
43	2l	119/132 (90%)	110 (92%)	9 (8%)	0	100	100
44	1m	114/126 (90%)	101 (89%)	13 (11%)	0	100	100
44	2m	112/126 (89%)	99 (88%)	11 (10%)	2 (2%)	8	28
45	1n	58/61 (95%)	53 (91%)	5 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	2n	58/61 (95%)	51 (88%)	5 (9%)	2 (3%)	3	13
46	1o	86/89 (97%)	81 (94%)	4 (5%)	1 (1%)	13	39
46	2o	86/89 (97%)	81 (94%)	4 (5%)	1 (1%)	13	39
47	1p	80/88 (91%)	70 (88%)	8 (10%)	2 (2%)	5	19
47	2p	80/88 (91%)	72 (90%)	8 (10%)	0	100	100
48	1q	97/105 (92%)	87 (90%)	8 (8%)	2 (2%)	7	23
48	2q	97/105 (92%)	88 (91%)	8 (8%)	1 (1%)	15	44
49	1r	66/88 (75%)	62 (94%)	4 (6%)	0	100	100
49	2r	66/88 (75%)	64 (97%)	2 (3%)	0	100	100
50	1s	81/93 (87%)	68 (84%)	12 (15%)	1 (1%)	13	39
50	2s	81/93 (87%)	70 (86%)	10 (12%)	1 (1%)	13	39
51	1t	94/106 (89%)	86 (92%)	5 (5%)	3 (3%)	4	13
51	2t	96/106 (91%)	89 (93%)	5 (5%)	2 (2%)	7	23
52	1u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
52	2u	21/27 (78%)	17 (81%)	4 (19%)	0	100	100
53	1y	95/113 (84%)	94 (99%)	1 (1%)	0	100	100
53	2y	94/113 (83%)	85 (90%)	7 (7%)	2 (2%)	7	23
All	All	11629/12354 (94%)	10708 (92%)	812 (7%)	109 (1%)	17	46

All (109) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
6	1G	47	LYS
6	1G	50	ALA
26	14	47	GLN
33	1b	126	GLU
36	1e	96	PRO
41	1j	55	LYS
5	2F	130	ALA
7	2H	126	PRO
26	24	62	ARG
33	2b	17	PHE
33	2b	20	GLU
34	2c	4	LYS
41	2j	79	ARG

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Mol	Chain	Res	Type
42	2k	106	LYS
7	1H	92	ILE
7	1H	159	GLU
14	1S	59	LYS
19	1X	94	GLY
26	14	45	GLY
33	1b	127	ILE
41	1j	77	PRO
48	1q	68	ARG
6	2G	117	PHE
8	2I	10	GLU
19	2X	94	GLY
21	2Z	156	LYS
21	2Z	169	GLU
35	2d	156	GLU
36	2e	98	THR
38	2g	32	ARG
51	2t	100	ILE
12	1Q	59	ARG
26	14	39	CYS
33	1b	17	PHE
33	1b	21	ARG
33	1b	231	GLU
35	1d	167	GLY
47	1p	28	ARG
50	1s	12	ASP
6	2G	48	GLU
7	2H	48	GLY
8	2I	116	LEU
11	2P	36	LYS
12	2Q	59	ARG
26	24	53	GLU
33	2b	88	ALA
37	2f	38	GLU
38	2g	7	ALA
38	2g	55	GLY
40	2i	43	ALA
42	2k	15	ALA
44	2m	7	VAL
44	2m	23	TYR
45	2n	25	VAL
50	2s	29	ARG

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Mol	Chain	Res	Type
53	2y	33	HIS
4	1E	28	ALA
4	1E	52	LEU
19	1X	67	GLY
20	1Y	103	GLY
36	1e	97	GLY
41	1j	78	ASN
41	1j	82	ILE
51	1t	99	LEU
4	2E	28	ALA
4	2E	52	LEU
6	2G	81	LYS
33	2b	9	GLU
33	2b	95	GLN
34	2c	3	ASN
34	2c	12	LEU
38	2g	131	LYS
40	2i	54	ASP
40	2i	96	LEU
51	2t	47	GLY
26	14	60	GLN
33	1b	9	GLU
33	1b	20	GLU
33	1b	125	PRO
42	1k	105	VAL
48	1q	67	LYS
6	2G	78	SER
11	2P	122	PRO
15	2T	127	ALA
26	24	54	GLY
33	2b	125	PRO
40	2i	44	VAL
45	2n	14	PRO
48	2q	49	GLU
53	2y	36	ASN
6	1G	84	LYS
14	1S	94	TYR
51	1t	47	GLY
33	2b	227	GLY
34	2c	41	GLY
41	2j	39	PRO
26	24	50	VAL

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Mol	Chain	Res	Type
46	2o	19	PRO
17	1V	79	VAL
39	1h	83	ILE
51	1t	100	ILE
41	2j	77	PRO
39	1h	51	VAL
41	1j	91	PRO
46	1o	86	GLY
47	1p	46	PRO
21	2Z	90	VAL
4	2E	71	GLY

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	214/218 (98%)	197 (92%)	17 (8%)	12	34
3	2D	215/218 (99%)	205 (95%)	10 (5%)	26	59
4	1E	164/166 (99%)	156 (95%)	8 (5%)	25	57
4	2E	164/166 (99%)	154 (94%)	10 (6%)	18	48
5	1F	160/166 (96%)	144 (90%)	16 (10%)	7	22
5	2F	159/166 (96%)	146 (92%)	13 (8%)	11	33
6	1G	144/156 (92%)	133 (92%)	11 (8%)	13	36
6	2G	142/156 (91%)	129 (91%)	13 (9%)	9	27
7	1H	144/148 (97%)	135 (94%)	9 (6%)	18	46
7	2H	143/148 (97%)	125 (87%)	18 (13%)	4	14
8	1I	111/124 (90%)	94 (85%)	17 (15%)	2	8
8	2I	108/124 (87%)	97 (90%)	11 (10%)	7	22
9	1N	119/119 (100%)	112 (94%)	7 (6%)	19	49
9	2N	118/119 (99%)	116 (98%)	2 (2%)	60	87
10	1O	100/100 (100%)	95 (95%)	5 (5%)	24	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	2O	100/100 (100%)	95 (95%)	5 (5%)	24	56
11	1P	115/116 (99%)	109 (95%)	6 (5%)	23	55
11	2P	115/116 (99%)	110 (96%)	5 (4%)	29	62
12	1Q	111/111 (100%)	102 (92%)	9 (8%)	11	33
12	2Q	111/111 (100%)	104 (94%)	7 (6%)	18	46
13	1R	101/101 (100%)	92 (91%)	9 (9%)	9	28
13	2R	101/101 (100%)	95 (94%)	6 (6%)	19	49
14	1S	87/88 (99%)	82 (94%)	5 (6%)	20	50
14	2S	85/88 (97%)	76 (89%)	9 (11%)	6	20
15	1T	115/127 (91%)	110 (96%)	5 (4%)	29	62
15	2T	113/127 (89%)	107 (95%)	6 (5%)	22	54
16	1U	93/94 (99%)	84 (90%)	9 (10%)	8	24
16	2U	93/94 (99%)	85 (91%)	8 (9%)	10	30
17	1V	81/82 (99%)	74 (91%)	7 (9%)	10	30
17	2V	80/82 (98%)	72 (90%)	8 (10%)	7	22
18	1W	90/92 (98%)	86 (96%)	4 (4%)	28	61
18	2W	90/92 (98%)	85 (94%)	5 (6%)	21	51
19	1X	77/78 (99%)	70 (91%)	7 (9%)	9	27
19	2X	77/78 (99%)	71 (92%)	6 (8%)	12	35
20	1Y	86/91 (94%)	80 (93%)	6 (7%)	15	40
20	2Y	86/91 (94%)	78 (91%)	8 (9%)	9	26
21	1Z	169/179 (94%)	159 (94%)	10 (6%)	19	49
21	2Z	165/179 (92%)	154 (93%)	11 (7%)	16	43
22	10	61/67 (91%)	58 (95%)	3 (5%)	25	57
22	20	61/67 (91%)	58 (95%)	3 (5%)	25	57
23	11	79/83 (95%)	75 (95%)	4 (5%)	24	55
23	21	81/83 (98%)	77 (95%)	4 (5%)	25	57
24	12	65/67 (97%)	60 (92%)	5 (8%)	13	35
24	22	66/67 (98%)	62 (94%)	4 (6%)	18	48
25	13	51/52 (98%)	45 (88%)	6 (12%)	5	16
25	23	50/52 (96%)	44 (88%)	6 (12%)	5	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	14	58/63 (92%)	50 (86%)	8 (14%)	3	11
26	24	54/63 (86%)	47 (87%)	7 (13%)	4	13
27	15	51/52 (98%)	48 (94%)	3 (6%)	19	49
27	25	50/52 (96%)	47 (94%)	3 (6%)	19	48
28	16	51/52 (98%)	47 (92%)	4 (8%)	12	35
28	26	50/52 (96%)	45 (90%)	5 (10%)	7	22
29	17	41/42 (98%)	41 (100%)	0	100	100
29	27	41/42 (98%)	41 (100%)	0	100	100
30	18	54/55 (98%)	51 (94%)	3 (6%)	21	51
30	28	54/55 (98%)	49 (91%)	5 (9%)	9	26
31	19	34/34 (100%)	34 (100%)	0	100	100
31	29	34/34 (100%)	33 (97%)	1 (3%)	42	76
33	1b	191/220 (87%)	172 (90%)	19 (10%)	8	23
33	2b	187/220 (85%)	166 (89%)	21 (11%)	6	18
34	1c	144/188 (77%)	134 (93%)	10 (7%)	15	41
34	2c	140/188 (74%)	130 (93%)	10 (7%)	14	39
35	1d	171/181 (94%)	153 (90%)	18 (10%)	7	20
35	2d	172/181 (95%)	153 (89%)	19 (11%)	6	19
36	1e	114/123 (93%)	107 (94%)	7 (6%)	18	48
36	2e	114/123 (93%)	106 (93%)	8 (7%)	15	40
37	1f	85/90 (94%)	76 (89%)	9 (11%)	6	20
37	2f	85/90 (94%)	79 (93%)	6 (7%)	14	39
38	1g	120/127 (94%)	110 (92%)	10 (8%)	11	32
38	2g	119/127 (94%)	114 (96%)	5 (4%)	30	63
39	1h	116/119 (98%)	106 (91%)	10 (9%)	10	30
39	2h	114/119 (96%)	105 (92%)	9 (8%)	12	34
40	1i	91/99 (92%)	81 (89%)	10 (11%)	6	19
40	2i	88/99 (89%)	78 (89%)	10 (11%)	5	18
41	1j	68/92 (74%)	62 (91%)	6 (9%)	10	29
41	2j	68/92 (74%)	59 (87%)	9 (13%)	4	12
42	1k	83/99 (84%)	78 (94%)	5 (6%)	19	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	2k	83/99 (84%)	77 (93%)	6 (7%)	14	38
43	1l	96/108 (89%)	93 (97%)	3 (3%)	40	74
43	2l	96/108 (89%)	94 (98%)	2 (2%)	53	84
44	1m	90/101 (89%)	84 (93%)	6 (7%)	16	43
44	2m	87/101 (86%)	79 (91%)	8 (9%)	9	27
45	1n	49/50 (98%)	45 (92%)	4 (8%)	11	33
45	2n	49/50 (98%)	45 (92%)	4 (8%)	11	33
46	1o	78/80 (98%)	75 (96%)	3 (4%)	33	67
46	2o	78/80 (98%)	75 (96%)	3 (4%)	33	67
47	1p	69/74 (93%)	62 (90%)	7 (10%)	7	22
47	2p	68/74 (92%)	59 (87%)	9 (13%)	4	12
48	1q	94/97 (97%)	90 (96%)	4 (4%)	29	62
48	2q	94/97 (97%)	88 (94%)	6 (6%)	17	45
49	1r	59/77 (77%)	56 (95%)	3 (5%)	24	55
49	2r	59/77 (77%)	57 (97%)	2 (3%)	37	71
50	1s	68/80 (85%)	61 (90%)	7 (10%)	7	21
50	2s	67/80 (84%)	55 (82%)	12 (18%)	2	5
51	1t	71/82 (87%)	64 (90%)	7 (10%)	8	23
51	2t	70/82 (85%)	61 (87%)	9 (13%)	4	13
52	1u	18/22 (82%)	17 (94%)	1 (6%)	21	51
52	2u	18/22 (82%)	16 (89%)	2 (11%)	6	19
53	1y	82/98 (84%)	79 (96%)	3 (4%)	34	68
53	2y	79/98 (81%)	74 (94%)	5 (6%)	18	46
All	All	9524/10260 (93%)	8805 (92%)	719 (8%)	13	37

All (719) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	3	VAL
3	1D	37	LEU
3	1D	39	LYS
3	1D	54	ARG
3	1D	61	LEU
3	1D	99	ASP

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Mol	Chain	Res	Type
3	1D	106	ILE
3	1D	111	LEU
3	1D	126	GLN
3	1D	140	THR
3	1D	141	VAL
3	1D	142	VAL
3	1D	155	LEU
3	1D	183	ARG
3	1D	193	VAL
3	1D	211	ARG
3	1D	229	VAL
4	1E	12	THR
4	1E	75	VAL
4	1E	77	ILE
4	1E	89	ASP
4	1E	113	PHE
4	1E	116	VAL
4	1E	119	ARG
4	1E	184	VAL
5	1F	18	ARG
5	1F	53	THR
5	1F	57	VAL
5	1F	74	ARG
5	1F	110	LEU
5	1F	132	VAL
5	1F	140	LEU
5	1F	151	SER
5	1F	158	THR
5	1F	170	LEU
5	1F	183	VAL
5	1F	189	THR
5	1F	191	ARG
5	1F	192	LEU
5	1F	197	ASP
5	1F	201	VAL
6	1G	3	LEU
6	1G	7	LEU
6	1G	43	LEU
6	1G	45	GLU
6	1G	52	ILE
6	1G	53	LEU
6	1G	86	MET

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Mol	Chain	Res	Type
6	1G	140	ILE
6	1G	153	ARG
6	1G	159	VAL
6	1G	167	GLU
7	1H	15	VAL
7	1H	18	GLU
7	1H	40	GLU
7	1H	52	VAL
7	1H	56	SER
7	1H	107	VAL
7	1H	119	GLU
7	1H	134	SER
7	1H	155	SER
8	1I	5	LEU
8	1I	9	LEU
8	1I	10	GLU
8	1I	21	VAL
8	1I	25	TYR
8	1I	38	LEU
8	1I	42	SER
8	1I	43	ASN
8	1I	44	LEU
8	1I	60	GLU
8	1I	75	LEU
8	1I	92	VAL
8	1I	101	LEU
8	1I	103	ARG
8	1I	107	VAL
8	1I	109	ILE
8	1I	116	LEU
9	1N	5	VAL
9	1N	33	LEU
9	1N	34	LEU
9	1N	48	MET
9	1N	99	LEU
9	1N	133	GLN
9	1N	138	LEU
10	1O	12	ASP
10	1O	28	SER
10	1O	53	LYS
10	1O	70	LYS
10	1O	98	VAL

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Mol	Chain	Res	Type
11	1P	56	SER
11	1P	59	LEU
11	1P	71	VAL
11	1P	99	LEU
11	1P	133	SER
11	1P	135	LEU
12	1Q	6	ARG
12	1Q	7	MET
12	1Q	21	THR
12	1Q	55	VAL
12	1Q	59	ARG
12	1Q	60	ARG
12	1Q	101	ARG
12	1Q	109	VAL
12	1Q	110	THR
13	1R	6	SER
13	1R	36	THR
13	1R	54	LEU
13	1R	67	LEU
13	1R	73	VAL
13	1R	75	LEU
13	1R	96	ARG
13	1R	100	LEU
13	1R	102	GLU
14	1S	46	VAL
14	1S	50	SER
14	1S	52	SER
14	1S	59	LYS
14	1S	85	VAL
15	1T	28	VAL
15	1T	34	VAL
15	1T	65	LYS
15	1T	67	SER
15	1T	128	GLU
16	1U	5	LYS
16	1U	8	VAL
16	1U	52	ARG
16	1U	74	LEU
16	1U	77	SER
16	1U	78	THR
16	1U	83	LEU
16	1U	104	GLN

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Mol	Chain	Res	Type
16	1U	108	GLU
17	1V	21	ARG
17	1V	32	THR
17	1V	52	VAL
17	1V	61	VAL
17	1V	62	LEU
17	1V	72	VAL
17	1V	79	VAL
18	1W	11	ARG
18	1W	17	VAL
18	1W	67	ASP
18	1W	100	THR
19	1X	23	GLU
19	1X	35	THR
19	1X	52	VAL
19	1X	60	ARG
19	1X	68	ARG
19	1X	81	VAL
19	1X	95	LEU
20	1Y	9	LYS
20	1Y	14	LEU
20	1Y	43	ASN
20	1Y	72	VAL
20	1Y	99	CYS
20	1Y	107	ASP
21	1Z	41	LEU
21	1Z	42	VAL
21	1Z	61	LEU
21	1Z	80	ARG
21	1Z	86	VAL
21	1Z	118	GLN
21	1Z	126	VAL
21	1Z	129	SER
21	1Z	150	LEU
21	1Z	170	THR
22	10	55	ARG
22	10	68	GLU
22	10	74	ARG
23	11	21	ARG
23	11	30	VAL
23	11	46	LEU
23	11	95	LEU

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Mol	Chain	Res	Type
24	12	3	LEU
24	12	32	LEU
24	12	45	SER
24	12	53	LEU
24	12	70	GLN
25	13	6	VAL
25	13	8	LEU
25	13	23	LEU
25	13	54	VAL
25	13	56	VAL
25	13	58	VAL
26	14	3	GLU
26	14	10	VAL
26	14	49	PHE
26	14	50	VAL
26	14	52	THR
26	14	61	ARG
26	14	63	TYR
26	14	65	ASP
27	15	6	VAL
27	15	16	ARG
27	15	58	LEU
28	16	5	VAL
28	16	6	ARG
28	16	48	VAL
28	16	52	VAL
30	18	30	ARG
30	18	31	HIS
30	18	34	TRP
33	1b	7	VAL
33	1b	15	VAL
33	1b	19	HIS
33	1b	44	LEU
33	1b	80	ILE
33	1b	93	VAL
33	1b	96	ARG
33	1b	103	THR
33	1b	106	LYS
33	1b	107	THR
33	1b	111	ARG
33	1b	122	PHE
33	1b	133	LYS

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Mol	Chain	Res	Type
33	1b	160	ASP
33	1b	168	THR
33	1b	189	ASP
33	1b	212	GLN
33	1b	213	LEU
33	1b	233	SER
34	1c	26	LYS
34	1c	33	LEU
34	1c	36	ASP
34	1c	70	VAL
34	1c	103	VAL
34	1c	105	GLU
34	1c	115	LEU
34	1c	128	PHE
34	1c	144	SER
34	1c	154	SER
35	1d	19	LEU
35	1d	61	LYS
35	1d	70	ILE
35	1d	77	ASN
35	1d	85	LYS
35	1d	86	LYS
35	1d	135	LEU
35	1d	152	SER
35	1d	157	LEU
35	1d	162	LEU
35	1d	166	LYS
35	1d	168	ARG
35	1d	182	LYS
35	1d	188	LEU
35	1d	194	LEU
35	1d	196	LEU
35	1d	204	ILE
35	1d	208	SER
36	1e	33	VAL
36	1e	41	VAL
36	1e	79	GLU
36	1e	137	GLU
36	1e	147	ASP
36	1e	151	LEU
36	1e	152	ARG
37	1f	10	LEU

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Mol	Chain	Res	Type
37	1f	16	GLN
37	1f	17	SER
37	1f	69	GLU
37	1f	70	ASP
37	1f	73	ASN
37	1f	74	ASP
37	1f	78	GLU
37	1f	98	LEU
38	1g	6	ARG
38	1g	10	ARG
38	1g	12	LEU
38	1g	13	GLN
38	1g	22	LEU
38	1g	59	LEU
38	1g	75	VAL
38	1g	104	LEU
38	1g	113	GLU
38	1g	144	MET
39	1h	24	THR
39	1h	26	VAL
39	1h	39	LEU
39	1h	51	VAL
39	1h	52	ASP
39	1h	54	ASP
39	1h	109	ILE
39	1h	120	THR
39	1h	121	ASP
39	1h	137	VAL
40	1i	17	VAL
40	1i	47	LEU
40	1i	50	LEU
40	1i	56	LEU
40	1i	64	THR
40	1i	65	VAL
40	1i	66	ARG
40	1i	81	ILE
40	1i	96	LEU
40	1i	108	VAL
41	1j	5	ARG
41	1j	34	VAL
41	1j	38	ILE
41	1j	67	THR

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Mol	Chain	Res	Type
41	1j	72	VAL
41	1j	81	THR
42	1k	16	SER
42	1k	25	TYR
42	1k	79	SER
42	1k	96	ARG
42	1k	105	VAL
43	1l	39	VAL
43	1l	84	LEU
43	1l	104	VAL
44	1m	4	ILE
44	1m	86	CYS
44	1m	90	LEU
44	1m	94	ARG
44	1m	102	ARG
44	1m	108	ARG
45	1n	3	ARG
45	1n	18	VAL
45	1n	22	THR
45	1n	33	VAL
46	1o	39	LEU
46	1o	64	ARG
46	1o	66	LEU
47	1p	11	SER
47	1p	20	VAL
47	1p	29	ASP
47	1p	42	ARG
47	1p	61	SER
47	1p	62	VAL
47	1p	67	THR
48	1q	45	HIS
48	1q	63	ARG
48	1q	66	SER
48	1q	97	SER
49	1r	39	VAL
49	1r	55	ARG
49	1r	65	ILE
50	1s	4	SER
50	1s	5	LEU
50	1s	9	VAL
50	1s	28	LYS
50	1s	38	SER

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Mol	Chain	Res	Type
50	1s	39	THR
50	1s	48	THR
51	1t	9	ASN
51	1t	23	ARG
51	1t	24	LEU
51	1t	60	GLU
51	1t	84	LEU
51	1t	91	LEU
51	1t	100	ILE
52	1u	17	THR
53	1y	3	MET
53	1y	23	ARG
53	1y	56	THR
3	2D	15	PHE
3	2D	27	THR
3	2D	37	LEU
3	2D	106	ILE
3	2D	111	LEU
3	2D	211	ARG
3	2D	229	VAL
3	2D	242	ARG
3	2D	253	GLN
3	2D	274	ARG
4	2E	12	THR
4	2E	40	GLU
4	2E	75	VAL
4	2E	77	ILE
4	2E	89	ASP
4	2E	113	PHE
4	2E	116	VAL
4	2E	119	ARG
4	2E	170	LEU
4	2E	184	VAL
5	2F	20	LEU
5	2F	74	ARG
5	2F	88	VAL
5	2F	106	ARG
5	2F	135	LYS
5	2F	140	LEU
5	2F	157	VAL
5	2F	170	LEU
5	2F	176	LEU

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Mol	Chain	Res	Type
5	2F	192	LEU
5	2F	197	ASP
5	2F	201	VAL
5	2F	203	GLN
6	2G	3	LEU
6	2G	7	LEU
6	2G	28	VAL
6	2G	36	LYS
6	2G	43	LEU
6	2G	49	ASP
6	2G	53	LEU
6	2G	75	LYS
6	2G	133	LEU
6	2G	138	GLN
6	2G	139	LEU
6	2G	145	THR
6	2G	164	GLU
7	2H	13	LYS
7	2H	33	LEU
7	2H	40	GLU
7	2H	43	VAL
7	2H	50	VAL
7	2H	52	VAL
7	2H	70	THR
7	2H	81	GLU
7	2H	88	LEU
7	2H	95	ARG
7	2H	98	LEU
7	2H	114	VAL
7	2H	123	PHE
7	2H	133	VAL
7	2H	136	ILE
7	2H	139	GLN
7	2H	167	GLU
7	2H	172	LYS
8	2I	38	LEU
8	2I	51	ILE
8	2I	68	LEU
8	2I	75	LEU
8	2I	76	THR
8	2I	85	GLU
8	2I	92	VAL

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Mol	Chain	Res	Type
8	2I	108	THR
8	2I	116	LEU
8	2I	129	THR
8	2I	142	VAL
9	2N	67	LEU
9	2N	87	LEU
10	2O	38	VAL
10	2O	53	LYS
10	2O	94	ARG
10	2O	96	THR
10	2O	98	VAL
11	2P	83	VAL
11	2P	86	LYS
11	2P	99	LEU
11	2P	125	VAL
11	2P	147	LEU
12	2Q	6	ARG
12	2Q	16	ARG
12	2Q	21	THR
12	2Q	22	LYS
12	2Q	60	ARG
12	2Q	106	VAL
12	2Q	109	VAL
13	2R	24	GLN
13	2R	36	THR
13	2R	54	LEU
13	2R	67	LEU
13	2R	100	LEU
13	2R	102	GLU
14	2S	8	GLU
14	2S	12	PHE
14	2S	19	LYS
14	2S	21	THR
14	2S	40	ILE
14	2S	50	SER
14	2S	52	SER
14	2S	78	LEU
14	2S	95	HIS
15	2T	6	LEU
15	2T	13	ARG
15	2T	34	VAL
15	2T	74	ARG

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Mol	Chain	Res	Type
15	2T	96	ARG
15	2T	107	ASP
16	2U	30	LYS
16	2U	31	SER
16	2U	55	ARG
16	2U	56	ASP
16	2U	74	LEU
16	2U	83	LEU
16	2U	104	GLN
16	2U	108	GLU
17	2V	7	THR
17	2V	35	LEU
17	2V	46	VAL
17	2V	51	VAL
17	2V	53	GLU
17	2V	62	LEU
17	2V	79	VAL
17	2V	82	ARG
18	2W	11	ARG
18	2W	13	SER
18	2W	17	VAL
18	2W	23	LEU
18	2W	37	ARG
19	2X	23	GLU
19	2X	52	VAL
19	2X	65	ARG
19	2X	66	LEU
19	2X	81	VAL
19	2X	95	LEU
20	2Y	2	ARG
20	2Y	3	VAL
20	2Y	5	MET
20	2Y	6	HIS
20	2Y	12	THR
20	2Y	72	VAL
20	2Y	85	VAL
20	2Y	99	CYS
21	2Z	24	LEU
21	2Z	31	ARG
21	2Z	33	LEU
21	2Z	72	ARG
21	2Z	74	VAL

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Mol	Chain	Res	Type
21	2Z	89	PHE
21	2Z	92	SER
21	2Z	107	THR
21	2Z	129	SER
21	2Z	140	ASP
21	2Z	185	GLU
22	20	11	ARG
22	20	74	ARG
22	20	82	ARG
23	21	5	CYS
23	21	35	THR
23	21	58	ILE
23	21	95	LEU
24	22	19	VAL
24	22	35	LEU
24	22	62	THR
24	22	70	GLN
25	23	6	VAL
25	23	18	ASP
25	23	23	LEU
25	23	31	LEU
25	23	54	VAL
25	23	56	VAL
26	24	33	VAL
26	24	50	VAL
26	24	52	THR
26	24	53	GLU
26	24	56	VAL
26	24	60	GLN
26	24	61	ARG
27	25	6	VAL
27	25	29	THR
27	25	55	ARG
28	26	6	ARG
28	26	13	CYS
28	26	14	THR
28	26	29	ASN
28	26	40	CYS
30	28	14	VAL
30	28	30	ARG
30	28	31	HIS
30	28	34	TRP

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Mol	Chain	Res	Type
30	28	50	LEU
31	29	7	VAL
33	2b	8	LYS
33	2b	24	TRP
33	2b	28	PHE
33	2b	39	ILE
33	2b	44	LEU
33	2b	52	GLU
33	2b	71	VAL
33	2b	79	ASP
33	2b	90	MET
33	2b	107	THR
33	2b	124	SER
33	2b	146	GLN
33	2b	160	ASP
33	2b	172	ILE
33	2b	187	LEU
33	2b	189	ASP
33	2b	195	ASP
33	2b	196	LEU
33	2b	220	ASP
33	2b	221	LEU
33	2b	233	SER
34	2c	3	ASN
34	2c	52	LEU
34	2c	72	LYS
34	2c	105	GLU
34	2c	127	ARG
34	2c	128	PHE
34	2c	152	ILE
34	2c	165	THR
34	2c	166	GLU
34	2c	195	VAL
35	2d	9	CYS
35	2d	12	CYS
35	2d	19	LEU
35	2d	52	SER
35	2d	59	ARG
35	2d	118	ARG
35	2d	122	ARG
35	2d	127	THR
35	2d	135	LEU

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Mol	Chain	Res	Type
35	2d	139	ARG
35	2d	150	GLU
35	2d	153	ARG
35	2d	157	LEU
35	2d	158	ILE
35	2d	166	LYS
35	2d	175	SER
35	2d	188	LEU
35	2d	202	LEU
35	2d	208	SER
36	2e	16	THR
36	2e	40	ARG
36	2e	41	VAL
36	2e	45	PHE
36	2e	79	GLU
36	2e	82	VAL
36	2e	137	GLU
36	2e	147	ASP
37	2f	17	SER
37	2f	45	LEU
37	2f	69	GLU
37	2f	71	ARG
37	2f	93	SER
37	2f	95	GLU
38	2g	24	THR
38	2g	75	VAL
38	2g	77	SER
38	2g	94	ARG
38	2g	115	ARG
39	2h	60	ARG
39	2h	69	ARG
39	2h	81	HIS
39	2h	83	ILE
39	2h	91	ARG
39	2h	97	VAL
39	2h	112	LEU
39	2h	113	SER
39	2h	114	THR
40	2i	3	GLN
40	2i	7	THR
40	2i	27	THR
40	2i	34	ASN

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Mol	Chain	Res	Type
40	2i	35	GLU
40	2i	64	THR
40	2i	81	ILE
40	2i	92	TYR
40	2i	108	VAL
40	2i	113	LYS
41	2j	13	HIS
41	2j	30	SER
41	2j	34	VAL
41	2j	47	PHE
41	2j	58	ASP
41	2j	72	VAL
41	2j	73	ASP
41	2j	84	GLN
41	2j	98	ILE
42	2k	30	VAL
42	2k	84	VAL
42	2k	103	LEU
42	2k	107	SER
42	2k	116	HIS
42	2k	117	ASN
43	2l	81	SER
43	2l	83	VAL
44	2m	3	ARG
44	2m	16	ASP
44	2m	49	THR
44	2m	62	ASN
44	2m	94	ARG
44	2m	96	LEU
44	2m	98	VAL
44	2m	116	THR
45	2n	18	VAL
45	2n	33	VAL
45	2n	57	ARG
45	2n	60	SER
46	2o	4	THR
46	2o	21	ASP
46	2o	39	LEU
47	2p	2	VAL
47	2p	20	VAL
47	2p	28	ARG
47	2p	38	TYR

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Mol	Chain	Res	Type
47	2p	47	ASP
47	2p	58	TYR
47	2p	62	VAL
47	2p	67	THR
47	2p	71	ARG
48	2q	13	ASP
48	2q	60	ILE
48	2q	63	ARG
48	2q	70	ARG
48	2q	86	GLU
48	2q	93	GLN
49	2r	42	ARG
49	2r	66	LEU
50	2s	16	LEU
50	2s	32	LYS
50	2s	33	THR
50	2s	40	ILE
50	2s	41	VAL
50	2s	47	HIS
50	2s	48	THR
50	2s	56	GLN
50	2s	69	HIS
50	2s	71	LEU
50	2s	77	THR
50	2s	79	THR
51	2t	10	LEU
51	2t	15	ARG
51	2t	45	GLN
51	2t	51	GLU
51	2t	62	LEU
51	2t	71	THR
51	2t	84	LEU
51	2t	86	ARG
51	2t	100	ILE
52	2u	8	THR
52	2u	15	ARG
53	2y	13	THR
53	2y	24	LEU
53	2y	32	THR
53	2y	60	VAL
53	2y	77	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (100)

such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	87	ASN
3	1D	164	GLN
3	1D	253	GLN
4	1E	48	GLN
5	1F	8	GLN
5	1F	69	HIS
5	1F	203	GLN
6	1G	26	GLN
6	1G	58	GLN
8	1I	104	GLN
8	1I	105	HIS
9	1N	8	GLN
13	1R	71	GLN
15	1T	123	GLN
19	1X	31	HIS
20	1Y	6	HIS
20	1Y	43	ASN
21	1Z	73	GLN
21	1Z	151	HIS
25	13	32	GLN
26	14	20	ASN
33	1b	40	HIS
34	1c	6	HIS
34	1c	37	GLN
34	1c	104	GLN
35	1d	77	ASN
35	1d	125	HIS
35	1d	129	ASN
36	1e	20	GLN
36	1e	56	GLN
37	1f	100	ASN
38	1g	28	ASN
38	1g	64	GLN
38	1g	122	HIS
38	1g	148	ASN
40	1i	3	GLN
40	1i	34	ASN
40	1i	73	GLN
40	1i	87	GLN
41	1j	13	HIS
41	1j	56	HIS
41	1j	84	GLN

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Mol	Chain	Res	Type
43	1l	99	HIS
44	1m	92	HIS
44	1m	106	ASN
46	1o	28	GLN
47	1p	16	HIS
48	1q	93	GLN
50	1s	69	HIS
50	1s	83	HIS
51	1t	16	HIS
53	1y	4	ASN
53	1y	38	HIS
3	2D	87	ASN
3	2D	253	GLN
5	2F	69	HIS
5	2F	75	HIS
8	2I	43	ASN
9	2N	133	GLN
10	2O	3	GLN
11	2P	70	GLN
12	2Q	57	HIS
12	2Q	123	HIS
13	2R	31	HIS
13	2R	71	GLN
15	2T	58	ASN
16	2U	81	HIS
17	2V	64	HIS
18	2W	61	ASN
19	2X	31	HIS
21	2Z	73	GLN
21	2Z	85	HIS
25	23	32	GLN
30	28	35	GLN
33	2b	78	GLN
34	2c	6	HIS
34	2c	28	GLN
35	2d	42	GLN
35	2d	77	ASN
35	2d	116	GLN
35	2d	123	HIS
36	2e	20	GLN
36	2e	56	GLN
38	2g	13	GLN

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Mol	Chain	Res	Type
38	2g	28	ASN
39	2h	81	HIS
40	2i	3	GLN
41	2j	68	HIS
41	2j	69	ASN
44	2m	62	ASN
44	2m	77	ASN
44	2m	106	ASN
45	2n	49	HIS
46	2o	13	GLN
46	2o	28	GLN
46	2o	62	GLN
47	2p	14	ASN
47	2p	16	HIS
50	2s	83	HIS
53	2y	18	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2862/2915 (98%)	421 (14%)	24 (0%)
1	2A	2855/2915 (97%)	467 (16%)	29 (1%)
2	1B	119/121 (98%)	10 (8%)	0
2	2B	119/121 (98%)	13 (10%)	0
32	1a	1494/1521 (98%)	258 (17%)	0
32	2a	1498/1521 (98%)	258 (17%)	0
All	All	8947/9114 (98%)	1427 (15%)	53 (0%)

All (1427) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	15	G
1	1A	27	G
1	1A	34	C
1	1A	45	C
1	1A	71	A
1	1A	74	A
1	1A	75	G
1	1A	95	G
1	1A	118	A
1	1A	119	A

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Mol	Chain	Res	Type
1	1A	120	U
1	1A	140	G
1	1A	181	A
1	1A	182	A
1	1A	188	G
1	1A	196	A
1	1A	199	A
1	1A	205	G
1	1A	215	G
1	1A	216	A
1	1A	221	A
1	1A	222	A
1	1A	228	A
1	1A	229	A
1	1A	233	A
1	1A	248	G
1	1A	264	C
1	1A	271(I)	G
1	1A	271(K)	U
1	1A	271(L)	U
1	1A	271(M)	G
1	1A	271(N)	U
1	1A	271(O)	C
1	1A	272(A)	U
1	1A	272(B)	G
1	1A	272(H)	C
1	1A	272(J)	C
1	1A	274	G
1	1A	275	G
1	1A	279	C
1	1A	308	G
1	1A	311	A
1	1A	330	A
1	1A	352	G
1	1A	363	G
1	1A	370	G
1	1A	372	G
1	1A	386	G
1	1A	396	G
1	1A	405	U
1	1A	411	G
1	1A	412	A

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Mol	Chain	Res	Type
1	1A	428	A
1	1A	448	U
1	1A	456	C
1	1A	457	A
1	1A	481	G
1	1A	505	A
1	1A	509	C
1	1A	528	A
1	1A	530	G
1	1A	531	C
1	1A	532	A
1	1A	533	G
1	1A	545	G
1	1A	549	G
1	1A	563	G
1	1A	568	U
1	1A	573	G
1	1A	575	A
1	1A	592	G
1	1A	603	A
1	1A	604	G
1	1A	607	U
1	1A	614(A)	U
1	1A	614(B)	G
1	1A	615	G
1	1A	621	A
1	1A	627	A
1	1A	637	A
1	1A	645	C
1	1A	652(E)	G
1	1A	652(U)	G
1	1A	654	A
1	1A	668	G
1	1A	669	G
1	1A	686	G
1	1A	730	C
1	1A	738	G
1	1A	775	G
1	1A	776	G
1	1A	782	A
1	1A	784	A
1	1A	785	G

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Mol	Chain	Res	Type
1	1A	790	C
1	1A	792	G
1	1A	805	G
1	1A	812	C
1	1A	827	U
1	1A	828	U
1	1A	855	G
1	1A	859	G
1	1A	866	A
1	1A	880	G
1	1A	881	G
1	1A	884	C
1	1A	885	C
1	1A	886	C
1	1A	887	A
1	1A	888	C
1	1A	889	C
1	1A	890	A
1	1A	896	A
1	1A	907	U
1	1A	910	A
1	1A	914	C
1	1A	915	C
1	1A	932	G
1	1A	938	G
1	1A	945	A
1	1A	946	G
1	1A	953	A
1	1A	958	U
1	1A	959	A
1	1A	961	C
1	1A	974	G
1	1A	975	C
1	1A	975(A)	G
1	1A	983	A
1	1A	996	A
1	1A	1012	U
1	1A	1013	C
1	1A	1021	A
1	1A	1025	G
1	1A	1026	U
1	1A	1033	U

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Mol	Chain	Res	Type
1	1A	1039	G
1	1A	1042	G
1	1A	1043	C
1	1A	1046	A
1	1A	1047	G
1	1A	1048	A
1	1A	1054	A
1	1A	1060	U
1	1A	1061	U
1	1A	1062	G
1	1A	1065	U
1	1A	1069	A
1	1A	1070	A
1	1A	1071	G
1	1A	1073	A
1	1A	1075	C
1	1A	1077	A
1	1A	1078	U
1	1A	1079	C
1	1A	1081	U
1	1A	1088	A
1	1A	1090	U
1	1A	1096	A
1	1A	1097	U
1	1A	1109	C
1	1A	1110	G
1	1A	1112	G
1	1A	1116	C
1	1A	1128	A
1	1A	1129	A
1	1A	1130	U
1	1A	1132	A
1	1A	1135	C
1	1A	1136	G
1	1A	1150	C
1	1A	1171	G
1	1A	1173	G
1	1A	1174	A
1	1A	1175	U
1	1A	1176	G
1	1A	1177	A
1	1A	1178	C

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Mol	Chain	Res	Type
1	1A	1195	G
1	1A	1210	A
1	1A	1211	U
1	1A	1218	C
1	1A	1236	G
1	1A	1241	A
1	1A	1250	G
1	1A	1253	A
1	1A	1256	G
1	1A	1271	G
1	1A	1272	A
1	1A	1273	U
1	1A	1276	A
1	1A	1281	G
1	1A	1300	U
1	1A	1301	A
1	1A	1345	C
1	1A	1352	U
1	1A	1359	A
1	1A	1360	A
1	1A	1365	A
1	1A	1370	C
1	1A	1384	A
1	1A	1385	G
1	1A	1416	G
1	1A	1417	C
1	1A	1420	U
1	1A	1421	G
1	1A	1428	C
1	1A	1445	A
1	1A	1450	G
1	1A	1452	A
1	1A	1455	G
1	1A	1460	A
1	1A	1467	C
1	1A	1471	A
1	1A	1479	G
1	1A	1482	G
1	1A	1493	C
1	1A	1508	A
1	1A	1509	C
1	1A	1509(A)	A

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Mol	Chain	Res	Type
1	1A	1525	G
1	1A	1542	A
1	1A	1543	C
1	1A	1556	C
1	1A	1558	A
1	1A	1569	A
1	1A	1578	U
1	1A	1581	G
1	1A	1584	C
1	1A	1586	A
1	1A	1608	A
1	1A	1609	A
1	1A	1610	A
1	1A	1634	A
1	1A	1648	C
1	1A	1654	A
1	1A	1658	C
1	1A	1674	G
1	1A	1700	A
1	1A	1701	A
1	1A	1703	G
1	1A	1721	G
1	1A	1722	A
1	1A	1739	U
1	1A	1740	G
1	1A	1756	G
1	1A	1758	G
1	1A	1762	A
1	1A	1763	G
1	1A	1764	G
1	1A	1773	A
1	1A	1780	A
1	1A	1782	C
1	1A	1791	A
1	1A	1800	C
1	1A	1801	G
1	1A	1811	G
1	1A	1812	A
1	1A	1816	G
1	1A	1829	A
1	1A	1839	G
1	1A	1847	A

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Mol	Chain	Res	Type
1	1A	1877	A
1	1A	1878	G
1	1A	1889	A
1	1A	1900	A
1	1A	1906	G
1	1A	1913	A
1	1A	1929	G
1	1A	1930	G
1	1A	1936	A
1	1A	1937	A
1	1A	1938	A
1	1A	1941	C
1	1A	1955	U
1	1A	1963	U
1	1A	1967	C
1	1A	1970	A
1	1A	1971	A
1	1A	1972	A
1	1A	1993	U
1	1A	1997	G
1	1A	2020	A
1	1A	2023	G
1	1A	2031	A
1	1A	2032	G
1	1A	2033	A
1	1A	2043	C
1	1A	2055	C
1	1A	2056	G
1	1A	2060	A
1	1A	2061	G
1	1A	2069	G
1	1A	2093	G
1	1A	2103	C
1	1A	2107	C
1	1A	2108	C
1	1A	2111	C
1	1A	2116	G
1	1A	2117	A
1	1A	2118	U
1	1A	2119	A
1	1A	2120	G
1	1A	2126	A

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Mol	Chain	Res	Type
1	1A	2127	G
1	1A	2132	U
1	1A	2133	G
1	1A	2134	A
1	1A	2135	A
1	1A	2138	C
1	1A	2139	C
1	1A	2141	G
1	1A	2142	C
1	1A	2144	U
1	1A	2145	C
1	1A	2146	C
1	1A	2148	G
1	1A	2152	G
1	1A	2153	G
1	1A	2158	A
1	1A	2159	G
1	1A	2161	C
1	1A	2170	A
1	1A	2173	A
1	1A	2176	A
1	1A	2178	C
1	1A	2186	G
1	1A	2187	G
1	1A	2190	G
1	1A	2192	G
1	1A	2198	A
1	1A	2206	G
1	1A	2207	G
1	1A	2208	A
1	1A	2225	A
1	1A	2235	G
1	1A	2238	G
1	1A	2239	G
1	1A	2240	C
1	1A	2268	A
1	1A	2273	A
1	1A	2283	C
1	1A	2287	A
1	1A	2289	G
1	1A	2305	A
1	1A	2308	G

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Mol	Chain	Res	Type
1	1A	2312	U
1	1A	2320	A
1	1A	2325	G
1	1A	2334	G
1	1A	2336	A
1	1A	2347	C
1	1A	2350	C
1	1A	2383	G
1	1A	2385	C
1	1A	2400	G
1	1A	2406	U
1	1A	2422	A
1	1A	2423	U
1	1A	2425	A
1	1A	2428	G
1	1A	2429	G
1	1A	2430	A
1	1A	2434	A
1	1A	2435	A
1	1A	2439	A
1	1A	2441	C
1	1A	2447	G
1	1A	2448	A
1	1A	2470	G
1	1A	2476	A
1	1A	2494	G
1	1A	2502	G
1	1A	2504	U
1	1A	2505	G
1	1A	2518	A
1	1A	2529	G
1	1A	2535	G
1	1A	2554	U
1	1A	2566	A
1	1A	2567	G
1	1A	2572	A
1	1A	2573	C
1	1A	2602	A
1	1A	2603	G
1	1A	2609	U
1	1A	2611	U
1	1A	2612	C

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Mol	Chain	Res	Type
1	1A	2629	A
1	1A	2630	G
1	1A	2646	C
1	1A	2654	A
1	1A	2689	U
1	1A	2690	C
1	1A	2702	U
1	1A	2703	C
1	1A	2712(A)	A
1	1A	2713	A
1	1A	2714	G
1	1A	2726	U
1	1A	2733	A
1	1A	2757	A
1	1A	2758	A
1	1A	2761	G
1	1A	2764	A
1	1A	2765	A
1	1A	2766	G
1	1A	2778	A
1	1A	2780	G
1	1A	2789	C
1	1A	2791	C
1	1A	2793	G
1	1A	2794	C
1	1A	2802	G
1	1A	2820	A
1	1A	2821	A
1	1A	2833	G
1	1A	2835	A
1	1A	2872	G
1	1A	2892	A
1	1A	2894	G
2	1B	5	C
2	1B	7	G
2	1B	13	A
2	1B	32	C
2	1B	45	A
2	1B	53	A
2	1B	56	G
2	1B	73	A
2	1B	106	G

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Mol	Chain	Res	Type
2	1B	110	G
32	1a	9	G
32	1a	32	A
32	1a	39	G
32	1a	47	C
32	1a	48	C
32	1a	50	A
32	1a	51	A
32	1a	61	G
32	1a	78	G
32	1a	79	G
32	1a	96	U
32	1a	101	A
32	1a	116	A
32	1a	121	C
32	1a	131	C
32	1a	144	G
32	1a	147	G
32	1a	163	C
32	1a	173	U
32	1a	174	C
32	1a	182	U
32	1a	195	A
32	1a	203	U
32	1a	204	U
32	1a	216	G
32	1a	220	G
32	1a	223	U
32	1a	247	G
32	1a	251	G
32	1a	258	G
32	1a	266	G
32	1a	267	C
32	1a	269	C
32	1a	289	G
32	1a	301	G
32	1a	306	G
32	1a	321	A
32	1a	328	C
32	1a	329	A
32	1a	332	G
32	1a	348	G

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Mol	Chain	Res	Type
32	1a	351	G
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	356	A
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	397	A
32	1a	398	C
32	1a	406	G
32	1a	412	A
32	1a	413	G
32	1a	423	G
32	1a	429	U
32	1a	439	A
32	1a	442	C
32	1a	443	C
32	1a	452	A
32	1a	458	C
32	1a	461	A
32	1a	470	C
32	1a	477	A
32	1a	484	G
32	1a	485	G
32	1a	496	A
32	1a	498	U
32	1a	505	G
32	1a	509	A
32	1a	510	A
32	1a	511	C
32	1a	518	C
32	1a	524	G
32	1a	532	A
32	1a	536	C
32	1a	547	A
32	1a	550	G
32	1a	559	A
32	1a	560	U
32	1a	561	U
32	1a	564	C
32	1a	572	A

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Mol	Chain	Res	Type
32	1a	573	A
32	1a	574	A
32	1a	576	G
32	1a	577	G
32	1a	596	C
32	1a	607	A
32	1a	619	U
32	1a	630	G
32	1a	631	G
32	1a	632	A
32	1a	653	A
32	1a	661	G
32	1a	665	A
32	1a	687	A
32	1a	688	G
32	1a	731	G
32	1a	734	G
32	1a	755	G
32	1a	768	A
32	1a	777	A
32	1a	793	U
32	1a	794	A
32	1a	796	C
32	1a	815	A
32	1a	816	A
32	1a	817	C
32	1a	821	G
32	1a	828	A
32	1a	829	G
32	1a	838	G
32	1a	840	C
32	1a	841	U
32	1a	848	C
32	1a	885	G
32	1a	902	G
32	1a	914	A
32	1a	916	G
32	1a	926	G
32	1a	927	G
32	1a	934	C
32	1a	935	A
32	1a	939	G

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Mol	Chain	Res	Type
32	1a	960	U
32	1a	961	U
32	1a	963	G
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	974	A
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	991	U
32	1a	992	U
32	1a	993	G
32	1a	996	A
32	1a	998	G
32	1a	1001	A
32	1a	1001(A)	G
32	1a	1003	G
32	1a	1004	A
32	1a	1005	A
32	1a	1009	G
32	1a	1022	G
32	1a	1023	G
32	1a	1024	G
32	1a	1025	U
32	1a	1026	G
32	1a	1027	C
32	1a	1028	C
32	1a	1029	C
32	1a	1030	C
32	1a	1030(A)	G
32	1a	1030(B)	C
32	1a	1030(C)	G
32	1a	1030(D)	A
32	1a	1032	G
32	1a	1033	G
32	1a	1034	G
32	1a	1036	G
32	1a	1037	C
32	1a	1039	C
32	1a	1044	A
32	1a	1046	A

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Mol	Chain	Res	Type
32	1a	1053	G
32	1a	1065	U
32	1a	1066	C
32	1a	1068	G
32	1a	1070	U
32	1a	1081	G
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1124	G
32	1a	1125	U
32	1a	1126	U
32	1a	1130	A
32	1a	1134	G
32	1a	1136	U
32	1a	1137	C
32	1a	1139	G
32	1a	1146	A
32	1a	1152	A
32	1a	1159	U
32	1a	1168	A
32	1a	1171	G
32	1a	1183	A
32	1a	1184	G
32	1a	1193	G
32	1a	1196	U
32	1a	1197	G
32	1a	1200	C
32	1a	1202	G
32	1a	1204	A
32	1a	1206	G
32	1a	1208	C
32	1a	1212	U
32	1a	1213	A
32	1a	1214	C
32	1a	1224	G
32	1a	1225	A
32	1a	1227	A
32	1a	1238	A
32	1a	1250	A
32	1a	1256	A
32	1a	1257	U

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Mol	Chain	Res	Type
32	1a	1258	G
32	1a	1270	C
32	1a	1278	U
32	1a	1280	A
32	1a	1286	A
32	1a	1287	A
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1312	G
32	1a	1317	C
32	1a	1319	A
32	1a	1320	C
32	1a	1322	C
32	1a	1338	G
32	1a	1340	A
32	1a	1344	C
32	1a	1346	A
32	1a	1347	G
32	1a	1353	G
32	1a	1360	A
32	1a	1363	C
32	1a	1370	G
32	1a	1381	U
32	1a	1397	C
32	1a	1398	A
32	1a	1419	G
32	1a	1422	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1442(B)	A
32	1a	1447	A
32	1a	1452	C
32	1a	1456	G
32	1a	1487	G
32	1a	1492	A
32	1a	1493	A
32	1a	1497	G
32	1a	1499	A
32	1a	1500	A
32	1a	1504	G
32	1a	1505	G

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Mol	Chain	Res	Type
32	1a	1506	U
32	1a	1507	A
32	1a	1517	G
32	1a	1520	G
32	1a	1529	G
32	1a	1530	G
32	1a	1531	A
1	2A	10	G
1	2A	15	G
1	2A	34	C
1	2A	45	C
1	2A	61	G
1	2A	63	U
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	78	A
1	2A	84	A
1	2A	88	G
1	2A	95	G
1	2A	99	U
1	2A	118	A
1	2A	119	A
1	2A	120	U
1	2A	140	G
1	2A	141	A
1	2A	157	U
1	2A	181	A
1	2A	182	A
1	2A	196	A
1	2A	198	C
1	2A	199	A
1	2A	205	G
1	2A	214	G
1	2A	215	G
1	2A	216	A
1	2A	221	A
1	2A	222	A
1	2A	229	A
1	2A	230	U
1	2A	232	G
1	2A	248	G

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Mol	Chain	Res	Type
1	2A	266	G
1	2A	271(K)	U
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	271(O)	C
1	2A	272(A)	U
1	2A	272(B)	G
1	2A	272(J)	C
1	2A	277	C
1	2A	278	A
1	2A	283	A
1	2A	303	U
1	2A	311	A
1	2A	324	A
1	2A	329	G
1	2A	330	A
1	2A	352	G
1	2A	370	G
1	2A	372	G
1	2A	386	G
1	2A	405	U
1	2A	411	G
1	2A	428	A
1	2A	444	C
1	2A	455	C
1	2A	457	A
1	2A	470	A
1	2A	477	A
1	2A	481	G
1	2A	504	U
1	2A	505	A
1	2A	508	G
1	2A	509	C
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	533	G
1	2A	545	G
1	2A	563	G
1	2A	568	U
1	2A	573	G

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Mol	Chain	Res	Type
1	2A	574	C
1	2A	575	A
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	614(B)	G
1	2A	615	G
1	2A	616	G
1	2A	627	A
1	2A	637	A
1	2A	645	C
1	2A	646	A
1	2A	652(B)	A
1	2A	652(C)	G
1	2A	652(U)	G
1	2A	653	A
1	2A	669	G
1	2A	686	G
1	2A	715	G
1	2A	726	G
1	2A	730	C
1	2A	752	A
1	2A	753	C
1	2A	774	A
1	2A	775	G
1	2A	776	G
1	2A	782	A
1	2A	784	A
1	2A	785	G
1	2A	792	G
1	2A	793	A
1	2A	794	G
1	2A	805	G
1	2A	812	C
1	2A	827	U
1	2A	857	C
1	2A	859	G
1	2A	874	G
1	2A	877	U
1	2A	880	G
1	2A	886	C
1	2A	887	A

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Mol	Chain	Res	Type
1	2A	888	C
1	2A	889	C
1	2A	890	A
1	2A	893	C
1	2A	896	A
1	2A	900	A
1	2A	901	A
1	2A	908	C
1	2A	910	A
1	2A	914	C
1	2A	917	A
1	2A	926	A
1	2A	932	G
1	2A	941	A
1	2A	945	A
1	2A	946	G
1	2A	959	A
1	2A	961	C
1	2A	968	G
1	2A	974	G
1	2A	975	C
1	2A	980	A
1	2A	983	A
1	2A	996	A
1	2A	1006	C
1	2A	1012	U
1	2A	1013	C
1	2A	1017	G
1	2A	1025	G
1	2A	1033	U
1	2A	1038	C
1	2A	1045	A
1	2A	1046	A
1	2A	1047	G
1	2A	1052	C
1	2A	1053	C
1	2A	1054	A
1	2A	1055	G
1	2A	1058	G
1	2A	1060	U
1	2A	1063	G
1	2A	1064	C

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Mol	Chain	Res	Type
1	2A	1065	U
1	2A	1066	U
1	2A	1067	A
1	2A	1068	G
1	2A	1069	A
1	2A	1070	A
1	2A	1071	G
1	2A	1073	A
1	2A	1074	G
1	2A	1076	C
1	2A	1078	U
1	2A	1079	C
1	2A	1082	U
1	2A	1083	U
1	2A	1084	A
1	2A	1085	A
1	2A	1086	A
1	2A	1088	A
1	2A	1089	G
1	2A	1090	U
1	2A	1091	G
1	2A	1092	C
1	2A	1093	G
1	2A	1095	A
1	2A	1096	A
1	2A	1098	A
1	2A	1108	U
1	2A	1109	C
1	2A	1110	G
1	2A	1112	G
1	2A	1116	C
1	2A	1117	G
1	2A	1118	C
1	2A	1122	G
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1142(A)	A
1	2A	1171	G
1	2A	1188	U
1	2A	1195	G
1	2A	1205	U

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Mol	Chain	Res	Type
1	2A	1211	U
1	2A	1212	G
1	2A	1220	A
1	2A	1248	G
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A
1	2A	1273	U
1	2A	1300	U
1	2A	1301	A
1	2A	1308	A
1	2A	1314	C
1	2A	1319	G
1	2A	1342	A
1	2A	1352	U
1	2A	1359	A
1	2A	1360	A
1	2A	1365	A
1	2A	1368	G
1	2A	1384	A
1	2A	1385	G
1	2A	1395	A
1	2A	1396	U
1	2A	1416	G
1	2A	1417	C
1	2A	1420	U
1	2A	1421	G
1	2A	1427	A
1	2A	1428	C
1	2A	1445	A
1	2A	1450	G
1	2A	1455	G
1	2A	1459	G
1	2A	1467	C
1	2A	1471	A
1	2A	1482	G
1	2A	1490	A
1	2A	1493	C
1	2A	1497	U
1	2A	1508	A
1	2A	1509	C

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Mol	Chain	Res	Type
1	2A	1509(A)	A
1	2A	1531	C
1	2A	1533	G
1	2A	1542	A
1	2A	1543	C
1	2A	1547	C
1	2A	1558	A
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1580	A
1	2A	1583	A
1	2A	1584	C
1	2A	1586	A
1	2A	1597	A
1	2A	1608	A
1	2A	1609	A
1	2A	1613	G
1	2A	1631	C
1	2A	1640	C
1	2A	1648	C
1	2A	1674	G
1	2A	1696	G
1	2A	1700	A
1	2A	1701	A
1	2A	1703	G
1	2A	1722	A
1	2A	1756	G
1	2A	1762	A
1	2A	1763	G
1	2A	1764	G
1	2A	1773	A
1	2A	1777	U
1	2A	1780	A
1	2A	1782	C
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1816	G
1	2A	1828	G
1	2A	1835	G
1	2A	1839	G

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Mol	Chain	Res	Type
1	2A	1847	A
1	2A	1848	A
1	2A	1877	A
1	2A	1878	G
1	2A	1900	A
1	2A	1906	G
1	2A	1914	C
1	2A	1927	A
1	2A	1929	G
1	2A	1930	G
1	2A	1938	A
1	2A	1955	U
1	2A	1963	U
1	2A	1965	C
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1993	U
1	2A	1997	G
1	2A	2020	A
1	2A	2023	G
1	2A	2031	A
1	2A	2032	G
1	2A	2033	A
1	2A	2043	C
1	2A	2055	C
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G
1	2A	2062	A
1	2A	2069	G
1	2A	2096	U
1	2A	2101	G
1	2A	2103	C
1	2A	2104	G
1	2A	2105	C
1	2A	2107	C
1	2A	2108	C
1	2A	2109	U
1	2A	2111	C
1	2A	2112	G

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Mol	Chain	Res	Type
1	2A	2116	G
1	2A	2117	A
1	2A	2118	U
1	2A	2119	A
1	2A	2120	G
1	2A	2123	G
1	2A	2126	A
1	2A	2127	G
1	2A	2129	C
1	2A	2130	U
1	2A	2131	G
1	2A	2132	U
1	2A	2133	G
1	2A	2134	A
1	2A	2135	A
1	2A	2136	C
1	2A	2141	G
1	2A	2145	C
1	2A	2146	C
1	2A	2147	G
1	2A	2148	G
1	2A	2150	U
1	2A	2151	G
1	2A	2152	G
1	2A	2156	G
1	2A	2157	G
1	2A	2158	A
1	2A	2159	G
1	2A	2161	C
1	2A	2163	C
1	2A	2165	G
1	2A	2168	G
1	2A	2172	U
1	2A	2173	A
1	2A	2178	C
1	2A	2186	G
1	2A	2187	G
1	2A	2189	U
1	2A	2192	G
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G

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Mol	Chain	Res	Type
1	2A	2208	A
1	2A	2218	U
1	2A	2219	G
1	2A	2225	A
1	2A	2235	G
1	2A	2239	G
1	2A	2269	A
1	2A	2275	C
1	2A	2278	A
1	2A	2283	C
1	2A	2287	A
1	2A	2289	G
1	2A	2294	C
1	2A	2305	A
1	2A	2308	G
1	2A	2311	A
1	2A	2312	U
1	2A	2320	A
1	2A	2321	G
1	2A	2322	A
1	2A	2325	G
1	2A	2334	G
1	2A	2335	A
1	2A	2336	A
1	2A	2343	C
1	2A	2347	C
1	2A	2350	C
1	2A	2354	G
1	2A	2366	A
1	2A	2369	A
1	2A	2372	G
1	2A	2379	G
1	2A	2383	G
1	2A	2385	C
1	2A	2396	G
1	2A	2406	U
1	2A	2410	G
1	2A	2414	G
1	2A	2422	A
1	2A	2425	A
1	2A	2429	G
1	2A	2430	A

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Mol	Chain	Res	Type
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2448	A
1	2A	2470	G
1	2A	2474	C
1	2A	2476	A
1	2A	2484	G
1	2A	2502	G
1	2A	2504	U
1	2A	2505	G
1	2A	2507	C
1	2A	2518	A
1	2A	2520	C
1	2A	2529	G
1	2A	2554	U
1	2A	2566	A
1	2A	2567	G
1	2A	2573	C
1	2A	2585	U
1	2A	2602	A
1	2A	2603	G
1	2A	2609	U
1	2A	2611	U
1	2A	2612	C
1	2A	2615	U
1	2A	2621	A
1	2A	2629	A
1	2A	2630	G
1	2A	2654	A
1	2A	2663	G
1	2A	2689	U
1	2A	2690	C
1	2A	2703	C
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2726	U
1	2A	2733	A
1	2A	2757	A
1	2A	2758	A
1	2A	2764	A
1	2A	2765	A

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Mol	Chain	Res	Type
1	2A	2778	A
1	2A	2818	G
1	2A	2820	A
1	2A	2821	A
1	2A	2835	A
1	2A	2849	U
1	2A	2872	G
1	2A	2880	C
1	2A	2886	G
1	2A	2894	G
1	2A	2895	U
1	2A	2897	U
2	2B	8	U
2	2B	9	G
2	2B	13	A
2	2B	30	C
2	2B	33	G
2	2B	35	U
2	2B	42	C
2	2B	56	G
2	2B	73	A
2	2B	84	C
2	2B	109	C
2	2B	110	G
2	2B	116	G
32	2a	5	U
32	2a	6	G
32	2a	7	G
32	2a	9	G
32	2a	22	G
32	2a	32	A
32	2a	39	G
32	2a	47	C
32	2a	48	C
32	2a	51	A
32	2a	61	G
32	2a	66	G
32	2a	79	G
32	2a	89	C
32	2a	101	A
32	2a	105	G
32	2a	116	A

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Mol	Chain	Res	Type
32	2a	121	C
32	2a	131	C
32	2a	151	A
32	2a	156	G
32	2a	163	C
32	2a	174	C
32	2a	176	C
32	2a	182	U
32	2a	189(E)	U
32	2a	195	A
32	2a	202	U
32	2a	203	U
32	2a	204	U
32	2a	216	G
32	2a	231	G
32	2a	247	G
32	2a	251	G
32	2a	258	G
32	2a	266	G
32	2a	267	C
32	2a	274	A
32	2a	279	A
32	2a	289	G
32	2a	298	A
32	2a	306	G
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	348	G
32	2a	351	G
32	2a	352	C
32	2a	353	A
32	2a	354	G
32	2a	367	U
32	2a	372	C
32	2a	373	A
32	2a	384	G
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	412	A
32	2a	413	G

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Mol	Chain	Res	Type
32	2a	423	G
32	2a	429	U
32	2a	439	A
32	2a	442	C
32	2a	452	A
32	2a	458	C
32	2a	461	A
32	2a	470	C
32	2a	471	G
32	2a	476	G
32	2a	482	A
32	2a	484	G
32	2a	485	G
32	2a	496	A
32	2a	498	U
32	2a	505	G
32	2a	506	G
32	2a	507	C
32	2a	508	C
32	2a	509	A
32	2a	510	A
32	2a	511	C
32	2a	518	C
32	2a	521	G
32	2a	527	7MG
32	2a	532	A
32	2a	533	A
32	2a	547	A
32	2a	559	A
32	2a	561	U
32	2a	564	C
32	2a	572	A
32	2a	573	A
32	2a	576	G
32	2a	577	G
32	2a	596	C
32	2a	630	G
32	2a	632	A
32	2a	650	G
32	2a	653	A
32	2a	665	A
32	2a	666	G

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Mol	Chain	Res	Type
32	2a	687	A
32	2a	688	G
32	2a	690	G
32	2a	695	A
32	2a	702	A
32	2a	703	G
32	2a	723	U
32	2a	731	G
32	2a	746	A
32	2a	749	C
32	2a	753	A
32	2a	755	G
32	2a	760	G
32	2a	770	C
32	2a	773	G
32	2a	774	G
32	2a	777	A
32	2a	793	U
32	2a	794	A
32	2a	815	A
32	2a	817	C
32	2a	819	A
32	2a	821	G
32	2a	828	A
32	2a	829	G
32	2a	840	C
32	2a	841	U
32	2a	848	C
32	2a	851	G
32	2a	859	A
32	2a	872	A
32	2a	875	C
32	2a	889	A
32	2a	902	G
32	2a	914	A
32	2a	926	G
32	2a	927	G
32	2a	931	C
32	2a	934	C
32	2a	935	A
32	2a	936	C
32	2a	942	G

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Mol	Chain	Res	Type
32	2a	960	U
32	2a	961	U
32	2a	966	M2G
32	2a	968	A
32	2a	969	A
32	2a	971	G
32	2a	972	C
32	2a	974	A
32	2a	975	A
32	2a	976	G
32	2a	977	A
32	2a	978	A
32	2a	984	C
32	2a	989	C
32	2a	992	U
32	2a	993	G
32	2a	994	A
32	2a	1003	G
32	2a	1004	A
32	2a	1005	A
32	2a	1006	C
32	2a	1009	G
32	2a	1015	A
32	2a	1020	U
32	2a	1022	G
32	2a	1023	G
32	2a	1025	U
32	2a	1026	G
32	2a	1027	C
32	2a	1028	C
32	2a	1030(A)	G
32	2a	1030(B)	C
32	2a	1041	A
32	2a	1044	A
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1071	C
32	2a	1081	G
32	2a	1094	G
32	2a	1095	U
32	2a	1101	A

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Mol	Chain	Res	Type
32	2a	1117	G
32	2a	1118	C
32	2a	1122	U
32	2a	1125	U
32	2a	1129	C
32	2a	1130	A
32	2a	1136	U
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G
32	2a	1147	C
32	2a	1152	A
32	2a	1157	A
32	2a	1159	U
32	2a	1183	A
32	2a	1184	G
32	2a	1194	U
32	2a	1196	U
32	2a	1197	G
32	2a	1204	A
32	2a	1211	U
32	2a	1212	U
32	2a	1213	A
32	2a	1215	G
32	2a	1224	G
32	2a	1227	A
32	2a	1238	A
32	2a	1250	A
32	2a	1256	A
32	2a	1257	U
32	2a	1258	G
32	2a	1260	C
32	2a	1270	C
32	2a	1278	U
32	2a	1279	A
32	2a	1281	U
32	2a	1282	C
32	2a	1285	A
32	2a	1287	A
32	2a	1300	G
32	2a	1302	U
32	2a	1303	C

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Mol	Chain	Res	Type
32	2a	1312	G
32	2a	1320	C
32	2a	1338	G
32	2a	1340	A
32	2a	1347	G
32	2a	1353	G
32	2a	1363	C
32	2a	1363(A)	A
32	2a	1368	G
32	2a	1370	G
32	2a	1397	C
32	2a	1406	U
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1445	C
32	2a	1446	U
32	2a	1447	A
32	2a	1492	A
32	2a	1494	G
32	2a	1497	G
32	2a	1499	A
32	2a	1503	A
32	2a	1504	G
32	2a	1506	U
32	2a	1507	A
32	2a	1517	G
32	2a	1520	G
32	2a	1528	U
32	2a	1529	G
32	2a	1530	G

All (53) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	195	A
1	1A	266	G
1	1A	278	A
1	1A	746	A
1	1A	839	U
1	1A	840	C
1	1A	887	A

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Mol	Chain	Res	Type
1	1A	895	U
1	1A	1047	G
1	1A	1065	U
1	1A	1067	A
1	1A	1175	U
1	1A	1176	G
1	1A	1210	A
1	1A	1275	A
1	1A	1442	G
1	1A	1608	A
1	1A	1653	G
1	1A	2126	A
1	1A	2288	A
1	1A	2430	A
1	1A	2689	U
1	1A	2756	U
1	1A	2893	G
1	2A	9	U
1	2A	195	A
1	2A	214	G
1	2A	266	G
1	2A	271(M)	G
1	2A	277	C
1	2A	752	A
1	2A	827	U
1	2A	840	C
1	2A	856	C
1	2A	900	A
1	2A	1053	C
1	2A	1057	A
1	2A	1065	U
1	2A	1067	A
1	2A	1073	A
1	2A	1210	A
1	2A	1420	U
1	2A	1442	G
1	2A	1491	G
1	2A	1992	G
1	2A	2126	A
1	2A	2171	A
1	2A	2172	U
1	2A	2321	G

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Mol	Chain	Res	Type
1	2A	2406	U
1	2A	2602	A
1	2A	2689	U
1	2A	2756	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	2MU	2A	2552	54,1	14,22,24	0.89	1 (7%)	14,31,36	0.78	1 (7%)
32	4OC	2a	1402	32	16,23,24	0.66	0	17,32,35	1.24	1 (5%)
1	5MC	1A	1962	54,1	15,22,23	1.36	1 (6%)	19,32,35	1.23	3 (15%)
1	5MC	2A	1962	54,1	15,22,23	1.26	1 (6%)	19,32,35	1.38	3 (15%)
32	UR3	1a	1498	32	14,22,23	0.71	0	15,32,35	0.70	0
1	5MU	1A	1939	1	15,22,23	1.09	1 (6%)	16,32,35	1.87	2 (12%)
32	MA6	1a	1518	32	19,26,27	0.81	0	18,38,41	1.41	2 (11%)
32	UR3	2a	1498	32	14,22,23	0.73	0	15,32,35	0.65	0
1	OMG	2A	2251	54,1	18,26,27	1.19	2 (11%)	20,38,41	2.13	6 (30%)
1	2MA	2A	2503	54,1	17,25,26	1.31	2 (11%)	19,37,40	1.97	3 (15%)
1	PSU	2A	1917	1	17,21,22	1.56	2 (11%)	20,30,33	3.13	6 (30%)
1	PSU	2A	1911	1	17,21,22	1.52	2 (11%)	20,30,33	3.17	6 (30%)
1	PSU	1A	2605	54,1	17,21,22	1.58	3 (17%)	20,30,33	3.09	6 (30%)
32	5MC	1a	1407	32	15,22,23	1.40	1 (6%)	19,32,35	1.21	3 (15%)
43	0TD	2l	92	43	4,9,10	3.08	1 (25%)	3,11,13	5.93	1 (33%)
32	5MC	2a	1400	32	15,22,23	1.29	1 (6%)	19,32,35	1.32	3 (15%)
32	2MG	1a	1207	32	19,26,27	1.25	2 (10%)	21,38,41	2.41	9 (42%)
32	5MC	2a	967	32	15,22,23	1.33	1 (6%)	19,32,35	1.28	3 (15%)
1	PSU	2A	2605	1	17,21,22	1.57	3 (17%)	20,30,33	3.32	6 (30%)
32	2MG	2a	1207	32	19,26,27	1.25	2 (10%)	21,38,41	2.13	6 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	5MC	1a	1404	32	15,22,23	1.31	1 (6%)	19,32,35	1.33	3 (15%)
32	7MG	2a	527	54,32	22,26,27	1.75	4 (18%)	28,39,42	2.73	9 (32%)
1	5MU	1A	1915	54,1	15,22,23	1.05	1 (6%)	16,32,35	2.04	1 (6%)
1	5MU	2A	1915	1	15,22,23	1.04	1 (6%)	16,32,35	1.99	1 (6%)
32	M2G	1a	966	32	20,27,28	1.38	3 (15%)	22,40,43	2.26	7 (31%)
32	MA6	2a	1518	32	19,26,27	0.79	0	18,38,41	1.43	2 (11%)
32	M2G	2a	966	54,32	20,27,28	1.42	3 (15%)	22,40,43	2.12	5 (22%)
1	4OC	1A	1920	1	15,22,24	0.65	0	17,31,35	1.37	2 (11%)
1	PSU	1A	1917	54,1	17,21,22	1.52	2 (11%)	20,30,33	3.16	5 (25%)
1	4OC	2A	1920	1	15,22,24	0.65	0	17,31,35	1.47	2 (11%)
32	5MC	1a	1400	32	15,22,23	1.35	1 (6%)	19,32,35	1.35	3 (15%)
1	5MU	2A	1939	1	15,22,23	1.17	1 (6%)	16,32,35	1.78	2 (12%)
32	5MC	2a	1407	32	15,22,23	1.32	1 (6%)	19,32,35	1.37	2 (10%)
1	2MA	1A	2503	54,1	17,25,26	1.35	2 (11%)	19,37,40	2.11	3 (15%)
43	0TD	1l	92	43	4,9,10	3.16	1 (25%)	3,11,13	4.31	1 (33%)
1	PSU	1A	1911	1	17,21,22	1.50	2 (11%)	20,30,33	3.05	7 (35%)
32	5MC	1a	967	32	15,22,23	1.26	1 (6%)	19,32,35	1.33	2 (10%)
1	5MC	1A	1942	1	15,22,23	1.25	1 (6%)	19,32,35	1.32	3 (15%)
32	MA6	1a	1519	32	19,26,27	0.83	0	18,38,41	1.37	2 (11%)
32	PSU	1a	516	54,32	17,21,22	1.50	3 (17%)	20,30,33	3.09	6 (30%)
1	5MC	2A	1942	1	15,22,23	1.32	1 (6%)	19,32,35	1.37	3 (15%)
32	5MC	2a	1404	32	15,22,23	1.33	1 (6%)	19,32,35	1.31	3 (15%)
1	2MU	1A	2552	54,1	14,22,24	0.88	1 (7%)	14,31,36	0.75	0
32	MA6	2a	1519	32	19,26,27	0.81	0	18,38,41	1.50	2 (11%)
32	7MG	1a	527	54,32	22,26,27	1.76	4 (18%)	28,39,42	2.74	8 (28%)
32	PSU	2a	516	54,32	17,21,22	1.52	3 (17%)	20,30,33	3.06	6 (30%)
32	4OC	1a	1402	32	16,23,24	0.61	0	17,32,35	1.15	1 (5%)
1	OMG	1A	2251	54,1	18,26,27	1.24	2 (11%)	20,38,41	2.19	6 (30%)

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	2MU	2A	2552	54,1	-	0/7/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	4OC	2a	1402	32	-	3/9/29/30	0/2/2/2
1	5MC	1A	1962	54,1	-	2/5/25/26	0/2/2/2
1	5MC	2A	1962	54,1	-	2/5/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/5/25/26	0/2/2/2
1	5MU	1A	1939	1	-	2/5/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/7/29/30	0/3/3/3
32	UR3	2a	1498	32	-	0/5/25/26	0/2/2/2
1	OMG	2A	2251	54,1	-	1/5/27/28	0/3/3/3
1	2MA	2A	2503	54,1	-	1/3/25/26	0/3/3/3
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	2605	54,1	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/5/25/26	0/2/2/2
43	0TD	2l	92	43	-	2/3/12/14	-
32	5MC	2a	1400	32	-	2/5/25/26	0/2/2/2
32	2MG	1a	1207	32	-	0/5/27/28	0/3/3/3
32	5MC	2a	967	32	-	0/5/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	0/5/27/28	0/3/3/3
32	5MC	1a	1404	32	-	0/5/25/26	0/2/2/2
32	7MG	2a	527	54,32	-	2/7/37/38	0/3/3/3
1	5MU	1A	1915	54,1	-	0/5/25/26	0/2/2/2
1	5MU	2A	1915	1	-	0/5/25/26	0/2/2/2
32	M2G	1a	966	32	-	1/7/29/30	0/3/3/3
32	MA6	2a	1518	32	-	0/7/29/30	0/3/3/3
32	M2G	2a	966	54,32	-	0/7/29/30	0/3/3/3
1	4OC	1A	1920	1	-	1/7/27/30	0/2/2/2
1	PSU	1A	1917	54,1	-	1/7/25/26	0/2/2/2
1	4OC	2A	1920	1	-	3/7/27/30	0/2/2/2
32	5MC	1a	1400	32	-	2/5/25/26	0/2/2/2
1	5MU	2A	1939	1	-	1/5/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/5/25/26	0/2/2/2
1	2MA	1A	2503	54,1	-	2/3/25/26	0/3/3/3
43	0TD	1l	92	43	-	1/3/12/14	-
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	1/5/25/26	0/2/2/2
1	5MC	1A	1942	1	-	0/5/25/26	0/2/2/2
32	MA6	1a	1519	32	-	1/7/29/30	0/3/3/3
32	PSU	1a	516	54,32	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/5/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	5MC	2a	1404	32	-	0/5/25/26	0/2/2/2
1	2MU	1A	2552	54,1	-	1/7/27/28	0/2/2/2
32	MA6	2a	1519	32	-	3/7/29/30	0/3/3/3
32	7MG	1a	527	54,32	-	1/7/37/38	0/3/3/3
32	PSU	2a	516	54,32	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
1	OMG	1A	2251	54,1	-	1/5/27/28	0/3/3/3

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-6.02	1.69	1.84
43	2l	92	0TD	CB-SB	-5.91	1.69	1.84
32	1a	1407	5MC	C5-C4	5.01	1.49	1.41
1	1A	1962	5MC	C5-C4	4.88	1.48	1.41
32	2a	967	5MC	C5-C4	4.83	1.48	1.41
32	2a	1404	5MC	C5-C4	4.80	1.48	1.41
32	1a	1400	5MC	C5-C4	4.78	1.48	1.41
1	2A	1942	5MC	C5-C4	4.71	1.48	1.41
32	2a	527	7MG	C6-C5	4.67	1.47	1.41
32	2a	1407	5MC	C5-C4	4.67	1.48	1.41
32	1a	1404	5MC	C5-C4	4.63	1.48	1.41
32	2a	1400	5MC	C5-C4	4.58	1.48	1.41
1	1A	2503	2MA	C6-C5	4.57	1.48	1.41
32	1a	967	5MC	C5-C4	4.55	1.48	1.41
32	1a	527	7MG	C5-C4	4.53	1.48	1.39
32	1a	527	7MG	C6-C5	4.52	1.47	1.41
1	2A	1962	5MC	C5-C4	4.46	1.48	1.41
1	1A	2605	PSU	C5-C1'	-4.45	1.48	1.52
1	1A	1942	5MC	C5-C4	4.38	1.48	1.41
32	2a	527	7MG	C5-C4	4.35	1.47	1.39
1	2A	2503	2MA	C6-C5	4.34	1.47	1.41
32	2a	966	M2G	C6-C5	4.27	1.48	1.41
1	1A	2251	OMG	C6-C5	4.24	1.48	1.41
32	2a	1207	2MG	C6-C5	4.23	1.48	1.41
1	2A	1917	PSU	C5-C1'	-4.22	1.48	1.52
32	1a	1207	2MG	C6-C5	4.21	1.48	1.41
32	1a	966	M2G	C6-C5	4.16	1.48	1.41
1	2A	2605	PSU	C5-C1'	-4.12	1.48	1.52
1	2A	2251	OMG	C6-C5	3.89	1.48	1.41
32	2a	516	PSU	C5-C1'	-3.87	1.48	1.52
1	2A	1911	PSU	C5-C1'	-3.80	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	1939	5MU	C4-C5	3.79	1.49	1.41
32	1a	527	7MG	C5-N7	-3.69	1.33	1.39
1	1A	1917	PSU	C5-C1'	-3.65	1.49	1.52
1	1A	1917	PSU	C4-C5	3.64	1.49	1.41
1	2A	1911	PSU	C4-C5	3.63	1.49	1.41
1	1A	1911	PSU	C5-C1'	-3.61	1.49	1.52
32	1a	516	PSU	C4-C5	3.59	1.49	1.41
1	1A	1911	PSU	C4-C5	3.57	1.49	1.41
32	2a	527	7MG	C5-N7	-3.53	1.33	1.39
32	1a	516	PSU	C5-C1'	-3.50	1.49	1.52
32	2a	516	PSU	C4-C5	3.41	1.48	1.41
1	2A	1917	PSU	C4-C5	3.40	1.48	1.41
1	2A	2605	PSU	C4-C5	3.39	1.48	1.41
32	2a	966	M2G	C2-N2	3.38	1.40	1.34
32	1a	966	M2G	C2-N2	3.37	1.40	1.34
1	1A	1939	5MU	C4-C5	3.37	1.48	1.41
1	1A	1915	5MU	C4-C5	3.28	1.48	1.41
1	2A	1915	5MU	C4-C5	3.26	1.48	1.41
1	1A	2605	PSU	C4-C5	3.01	1.47	1.41
32	2a	966	M2G	C5-C4	2.62	1.47	1.40
1	2A	2251	OMG	C5-C4	2.53	1.47	1.40
32	2a	1207	2MG	C5-C4	2.51	1.47	1.40
1	2A	2503	2MA	C5-C4	2.42	1.47	1.40
32	1a	1207	2MG	C5-C4	2.39	1.47	1.40
32	1a	527	7MG	C4-N9	-2.37	1.33	1.38
1	1A	2251	OMG	C5-C4	2.34	1.47	1.40
1	1A	2503	2MA	C5-C4	2.33	1.47	1.40
32	1a	966	M2G	C5-C4	2.29	1.47	1.40
32	2a	527	7MG	C4-N9	-2.26	1.34	1.38
1	1A	2605	PSU	C2-N3	-2.21	1.33	1.38
1	2A	2605	PSU	C2-N3	-2.20	1.33	1.38
32	2a	516	PSU	O4'-C1'	-2.16	1.41	1.44
32	1a	516	PSU	O4'-C1'	-2.07	1.41	1.44
1	1A	2552	2MU	C2-N3	-2.02	1.34	1.38
1	2A	2552	2MU	C2-N3	-2.00	1.34	1.38

All (167) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	2l	92	0TD	CSB-SB-CB	-10.20	81.80	101.85
1	2A	2605	PSU	N1-C2-N3	-9.05	121.24	128.43
32	1a	527	7MG	N3-C4-N9	8.96	138.42	126.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	527	7MG	N3-C4-N9	8.91	138.35	126.91
1	1A	1917	PSU	N1-C2-N3	-8.72	121.50	128.43
1	1A	2605	PSU	N1-C2-N3	-8.53	121.65	128.43
32	1a	516	PSU	N1-C2-N3	-8.50	121.68	128.43
1	2A	1911	PSU	N1-C2-N3	-8.48	121.69	128.43
1	2A	1917	PSU	N1-C2-N3	-8.47	121.70	128.43
32	2a	516	PSU	N1-C2-N3	-8.35	121.79	128.43
1	1A	1911	PSU	N1-C2-N3	-8.34	121.80	128.43
1	1A	1915	5MU	C4-N3-C2	7.55	121.52	115.14
43	1l	92	0TD	CSB-SB-CB	-7.36	87.38	101.85
1	2A	1915	5MU	C4-N3-C2	7.28	121.29	115.14
1	1A	1917	PSU	C4-N3-C2	7.07	121.11	115.14
32	1a	516	PSU	C4-N3-C2	6.94	121.00	115.14
1	2A	1911	PSU	C4-N3-C2	6.94	121.00	115.14
1	2A	2605	PSU	C4-N3-C2	6.93	120.99	115.14
1	1A	2503	2MA	C2-N3-C4	6.86	121.10	115.52
1	2A	1917	PSU	C4-N3-C2	6.73	120.82	115.14
32	2a	516	PSU	C4-N3-C2	6.63	120.74	115.14
1	1A	1911	PSU	C4-N3-C2	6.48	120.61	115.14
1	1A	1939	5MU	C4-N3-C2	6.35	120.50	115.14
1	1A	2605	PSU	C4-N3-C2	6.16	120.34	115.14
1	2A	1939	5MU	C4-N3-C2	6.05	120.25	115.14
1	2A	2503	2MA	C2-N3-C4	5.78	120.22	115.52
1	2A	1911	PSU	C5-C4-N3	-5.40	118.40	125.36
1	2A	1917	PSU	C5-C4-N3	-5.39	118.41	125.36
1	1A	1917	PSU	C5-C4-N3	-5.38	118.43	125.36
32	1a	516	PSU	C5-C4-N3	-5.37	118.44	125.36
32	2a	516	PSU	C5-C4-N3	-5.34	118.48	125.36
32	1a	966	M2G	C2-N3-C4	5.29	121.28	115.28
32	2a	527	7MG	N7-C8-N9	-5.29	95.82	103.38
1	1A	1911	PSU	C5-C4-N3	-5.25	118.59	125.36
32	2a	966	M2G	C6-N1-C2	5.22	122.39	116.18
1	2A	2503	2MA	C5-C6-N1	-5.13	117.68	123.06
32	2a	527	7MG	C5-C4-N3	-5.10	118.17	126.49
1	1A	2251	OMG	C2-N3-C4	5.09	121.17	115.36
32	1a	527	7MG	N7-C8-N9	-5.09	96.10	103.38
1	2A	2251	OMG	C2-N3-C4	5.03	121.11	115.36
1	2A	2605	PSU	C5-C4-N3	-5.02	118.90	125.36
32	1a	527	7MG	C5-C4-N3	-4.99	118.34	126.49
32	1a	966	M2G	C6-N1-C2	4.96	122.08	116.18
32	1a	1207	2MG	C2-N3-C4	4.87	120.81	115.28
32	2a	966	M2G	C2-N3-C4	4.87	120.81	115.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1518	MA6	N3-C2-N1	-4.87	121.07	128.68
32	2a	1519	MA6	N3-C2-N1	-4.77	121.22	128.68
1	1A	2605	PSU	C5-C4-N3	-4.73	119.26	125.36
32	2a	1207	2MG	C2-N3-C4	4.72	120.64	115.28
1	1A	2503	2MA	C5-C6-N1	-4.67	118.16	123.06
32	1a	1518	MA6	N3-C2-N1	-4.66	121.40	128.68
1	2A	1920	4OC	C2-N3-C4	4.55	120.95	116.34
1	1A	2605	PSU	C5-C6-N1	-4.53	118.87	124.44
32	2a	527	7MG	C6-N1-C2	4.46	123.01	115.93
32	1a	527	7MG	C6-N1-C2	4.44	122.99	115.93
32	1a	1519	MA6	N3-C2-N1	-4.43	121.75	128.68
32	1a	527	7MG	C6-C5-C4	4.43	119.95	115.20
1	2A	2605	PSU	C5-C1'-C2'	-4.38	107.50	115.32
1	2A	2605	PSU	C6-N1-C2	4.37	122.57	115.36
1	1A	1920	4OC	C2-N3-C4	4.36	120.76	116.34
1	1A	2605	PSU	C6-N1-C2	4.31	122.48	115.36
32	2a	1207	2MG	C5-C6-N1	-4.24	117.63	123.43
1	1A	1911	PSU	C6-N1-C2	4.21	122.30	115.36
32	2a	516	PSU	C5-C6-N1	-4.21	119.27	124.44
32	2a	966	M2G	C5-C6-N1	-4.21	117.68	123.43
1	1A	1917	PSU	C6-N1-C2	4.17	122.24	115.36
1	2A	2605	PSU	C5-C6-N1	-4.15	119.33	124.44
1	2A	2251	OMG	C6-N1-C2	4.14	122.51	115.93
32	2a	516	PSU	C6-N1-C2	4.14	122.19	115.36
32	1a	1207	2MG	C6-C5-C4	-4.13	116.85	120.80
32	1a	516	PSU	C6-N1-C2	4.11	122.14	115.36
32	2a	527	7MG	C6-C5-C4	4.10	119.61	115.20
1	2A	1917	PSU	C6-N1-C2	4.10	122.13	115.36
1	1A	1911	PSU	C5-C6-N1	-4.09	119.41	124.44
32	1a	1207	2MG	C5-C6-N1	-4.08	117.85	123.43
32	1a	966	M2G	C6-C5-C4	-4.07	116.91	120.80
32	1a	1207	2MG	C6-N1-C2	4.07	122.47	115.18
1	2A	2251	OMG	C5-C6-N1	-4.06	117.88	123.43
1	2A	1917	PSU	C5-C6-N1	-4.05	119.47	124.44
1	2A	1911	PSU	C6-N1-C2	4.04	122.03	115.36
32	2a	1207	2MG	C6-N1-C2	3.96	122.26	115.18
1	1A	2251	OMG	C6-N1-C2	3.92	122.16	115.93
1	1A	2251	OMG	C5-C6-N1	-3.91	118.09	123.43
32	1a	516	PSU	C5-C6-N1	-3.88	119.67	124.44
32	2a	1407	5MC	C2-N3-C4	3.88	120.70	116.02
32	1a	527	7MG	C5-C6-N1	-3.84	115.25	123.14
1	2A	1911	PSU	C5-C6-N1	-3.83	119.74	124.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1917	PSU	C5-C6-N1	-3.82	119.75	124.44
32	2a	1402	4OC	CM4-N4-C4	-3.78	119.72	122.97
32	1a	966	M2G	C5-C6-N1	-3.77	118.27	123.43
32	2a	967	5MC	C2-N3-C4	3.74	120.53	116.02
32	1a	967	5MC	C2-N3-C4	3.68	120.46	116.02
32	2a	527	7MG	C5-C6-N1	-3.63	115.69	123.14
32	1a	1400	5MC	C2-N3-C4	3.62	120.39	116.02
32	1a	1404	5MC	C2-N3-C4	3.58	120.34	116.02
32	2a	1404	5MC	C2-N3-C4	3.58	120.34	116.02
32	1a	1402	4OC	CM4-N4-C4	-3.53	119.93	122.97
32	1a	1207	2MG	CM2-N2-C2	-3.51	119.36	123.59
32	2a	1207	2MG	C6-C5-C4	-3.50	117.45	120.80
1	1A	1942	5MC	C2-N3-C4	3.49	120.23	116.02
1	1A	2251	OMG	C6-C5-C4	-3.49	117.47	120.80
1	2A	1942	5MC	C2-N3-C4	3.49	120.23	116.02
32	2a	966	M2G	C6-C5-C4	-3.46	117.49	120.80
1	2A	1911	PSU	C5-C1'-C2'	-3.45	109.16	115.32
1	2A	2251	OMG	N3-C2-N1	-3.44	122.64	127.22
32	2a	1400	5MC	C2-N3-C4	3.43	120.16	116.02
32	1a	1407	5MC	C2-N3-C4	3.33	120.04	116.02
1	1A	2251	OMG	N3-C2-N1	-3.33	122.79	127.22
32	2a	1519	MA6	C4-C5-N7	-3.30	105.96	109.40
1	2A	2251	OMG	C6-C5-C4	-3.28	117.67	120.80
1	1A	2605	PSU	C5-C1'-C2'	-3.27	109.48	115.32
1	1A	1962	5MC	C2-N3-C4	3.27	119.97	116.02
1	2A	1962	5MC	C2-N3-C4	3.23	119.92	116.02
1	1A	1939	5MU	C5-C6-N1	-3.09	118.86	122.19
1	1A	2251	OMG	C4-C5-N7	-3.03	106.24	109.40
1	2A	1962	5MC	N4-C4-N3	2.99	121.26	117.03
32	2a	1207	2MG	CM2-N2-C2	-2.97	120.01	123.59
32	1a	1518	MA6	C4-C5-N7	-2.96	106.31	109.40
32	1a	1519	MA6	C4-C5-N7	-2.90	106.38	109.40
32	1a	1207	2MG	C4-C5-N7	-2.88	106.40	109.40
32	2a	1518	MA6	C4-C5-N7	-2.88	106.40	109.40
1	2A	1939	5MU	C5-C6-N1	-2.85	119.12	122.19
1	2A	1917	PSU	C5-C1'-C2'	-2.82	110.28	115.32
32	1a	966	M2G	C4-C5-N7	-2.80	106.48	109.40
32	1a	966	M2G	N1-C2-N2	2.79	120.01	117.19
1	1A	2503	2MA	C4-C5-N7	-2.78	106.50	109.40
32	2a	527	7MG	C8-N7-C5	2.75	116.08	108.94
32	2a	1207	2MG	C4-C5-N7	-2.74	106.54	109.40
32	2a	1400	5MC	N4-C4-N3	2.73	120.90	117.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	966	M2G	C4-C5-N7	-2.70	106.59	109.40
1	2A	1942	5MC	N4-C4-N3	2.68	120.82	117.03
32	2a	1407	5MC	N4-C4-N3	2.63	120.75	117.03
32	1a	967	5MC	N4-C4-N3	2.62	120.73	117.03
32	1a	527	7MG	C8-N7-C5	2.61	115.73	108.94
32	1a	1404	5MC	N4-C4-N3	2.57	120.66	117.03
1	2A	1962	5MC	C5-C6-N1	-2.55	119.45	122.19
1	2A	1942	5MC	C5-C6-N1	-2.53	119.47	122.19
32	1a	1207	2MG	N2-C2-N1	2.52	119.39	116.96
32	1a	1400	5MC	C5-C6-N1	-2.52	119.48	122.19
1	1A	1942	5MC	N4-C4-N3	2.50	120.56	117.03
1	1A	1962	5MC	C5-C6-N1	-2.47	119.53	122.19
1	2A	2503	2MA	C4-C5-N7	-2.47	106.83	109.40
32	2a	1404	5MC	N4-C4-N3	2.42	120.45	117.03
32	2a	967	5MC	N4-C4-N3	2.41	120.44	117.03
32	2a	1400	5MC	C5-C6-N1	-2.41	119.60	122.19
32	1a	1400	5MC	N4-C4-N3	2.39	120.41	117.03
1	1A	1942	5MC	C5-C6-N1	-2.36	119.65	122.19
32	2a	1404	5MC	C5-C6-N1	-2.34	119.67	122.19
1	2A	1920	4OC	N4-C4-N3	2.33	120.18	116.49
32	1a	966	M2G	CM1-N2-C2	-2.33	119.07	121.29
32	1a	527	7MG	C5-C4-N9	-2.29	103.23	106.44
32	1a	1407	5MC	C5-C6-N1	-2.25	119.78	122.19
1	2A	2251	OMG	C4-C5-N7	-2.24	107.06	109.40
1	1A	1962	5MC	N4-C4-N3	2.24	120.20	117.03
32	1a	1207	2MG	O3'-C3'-C2'	2.20	118.92	111.82
1	1A	1920	4OC	N4-C4-N3	2.19	119.94	116.49
32	2a	516	PSU	O4'-C1'-C2'	2.17	108.18	104.66
32	1a	1404	5MC	C5-C6-N1	-2.17	119.86	122.19
32	2a	527	7MG	C5-C4-N9	-2.12	103.47	106.44
32	1a	1207	2MG	N3-C2-N1	-2.12	122.88	126.23
32	2a	527	7MG	C2-N3-C4	2.11	119.73	113.89
32	1a	1407	5MC	N4-C4-N3	2.10	120.01	117.03
32	2a	967	5MC	C5-C6-N1	-2.04	119.99	122.19
1	1A	1911	PSU	C5-C1'-C2'	-2.04	111.68	115.32
1	1A	1911	PSU	O4'-C1'-C2'	2.04	107.97	104.66
32	1a	516	PSU	O4'-C1'-C2'	2.03	107.94	104.66
1	2A	2552	2MU	C5-C4-N3	-2.01	118.88	123.31

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1A	1920	4OC	O4'-C1'-N1-C6
1	1A	1939	5MU	C2'-C1'-N1-C6
1	1A	1939	5MU	O4'-C1'-N1-C6
1	1A	1962	5MC	O4'-C1'-N1-C6
1	1A	1962	5MC	C2'-C1'-N1-C6
1	2A	1920	4OC	O4'-C1'-N1-C6
1	2A	1939	5MU	O4'-C1'-N1-C6
1	2A	1962	5MC	O4'-C1'-N1-C6
1	2A	1962	5MC	C2'-C1'-N1-C6
1	2A	2251	OMG	C1'-C2'-O2'-CM2
32	2a	527	7MG	C3'-C4'-C5'-O5'
32	2a	1400	5MC	O4'-C1'-N1-C6
32	2a	1400	5MC	C2'-C1'-N1-C6
32	2a	1519	MA6	O4'-C4'-C5'-O5'
43	2l	92	0TD	CG-CB-SB-CSB
32	2a	1402	4OC	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
32	2a	1402	4OC	C3'-C4'-C5'-O5'
32	2a	527	7MG	O4'-C4'-C5'-O5'
32	1a	1400	5MC	O4'-C4'-C5'-O5'
32	1a	1402	4OC	O4'-C4'-C5'-O5'
1	2A	2503	2MA	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C4'-C5'-O5'-P
1	1A	2251	OMG	C4'-C5'-O5'-P
32	2a	1402	4OC	C3'-C2'-O2'-CM2
32	1a	1400	5MC	C3'-C4'-C5'-O5'
43	2l	92	0TD	CA-CB-SB-CSB
32	1a	1519	MA6	O4'-C4'-C5'-O5'
1	1A	1917	PSU	C2'-C1'-C5-C6
1	1A	2552	2MU	O4'-C4'-C5'-O5'
32	1a	527	7MG	C3'-C4'-C5'-O5'
32	1a	967	5MC	O4'-C4'-C5'-O5'
1	2A	1920	4OC	C1'-C2'-O2'-CM2
1	2A	1920	4OC	C3'-C2'-O2'-CM2
32	1a	1402	4OC	C3'-C4'-C5'-O5'
1	1A	2503	2MA	C4'-C5'-O5'-P
1	1A	2503	2MA	O4'-C4'-C5'-O5'
43	1l	92	0TD	CG-CB-SB-CSB
32	1a	966	M2G	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2579 ligands modelled in this entry, 2566 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
56	MPD	1A	4056	-	7,7,7	0.31	0	9,10,10	0.25	0
56	MPD	2B	220	-	7,7,7	0.28	0	9,10,10	0.19	0
57	ARG	1B	228	-	7,11,11	0.22	0	6,13,13	0.40	0
59	SF4	1d	306	35	0,12,12	0.00	-	-		
57	ARG	1F	316	-	7,11,11	0.25	0	6,13,13	0.24	0
56	MPD	1T	207	-	7,7,7	0.27	0	9,10,10	0.22	0
55	YXM	1A	4055	-	42,43,43	2.99	6 (14%)	55,58,58	1.31	5 (9%)
56	MPD	2A	3760	-	7,7,7	0.29	0	9,10,10	0.29	0
55	YXM	2A	3758	-	42,43,43	2.82	7 (16%)	55,58,58	1.51	8 (14%)
59	SF4	2d	501	35	0,12,12	0.00	-	-		
56	MPD	2A	3759	-	7,7,7	0.27	0	9,10,10	0.26	0
56	MPD	18	102	-	7,7,7	0.23	0	9,10,10	0.21	0
56	MPD	1a	3280	-	7,7,7	0.34	0	9,10,10	0.32	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
56	MPD	1A	4056	-	-	2/5/5/5	-
56	MPD	2B	220	-	-	3/5/5/5	-
57	ARG	1B	228	-	-	1/7/11/11	-
59	SF4	1d	306	35	-	-	0/6/5/5
57	ARG	1F	316	-	-	4/7/11/11	-
56	MPD	1T	207	-	-	0/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	YXM	1A	4055	-	-	3/42/44/44	0/4/4/4
56	MPD	2A	3760	-	-	4/5/5/5	-
55	YXM	2A	3758	-	-	3/42/44/44	0/4/4/4
59	SF4	2d	501	35	-	-	0/6/5/5
56	MPD	2A	3759	-	-	0/5/5/5	-
56	MPD	18	102	-	-	2/5/5/5	-
56	MPD	1a	3280	-	-	2/5/5/5	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	1A	4055	YXM	OAK-NAG	14.51	1.47	1.22
55	2A	3758	YXM	OAK-NAG	13.83	1.46	1.22
55	2A	3758	YXM	CAB-CAH	-8.12	1.39	1.51
55	1A	4055	YXM	CAB-CAH	-7.56	1.40	1.51
55	1A	4055	YXM	PAV-CAY	-6.43	1.68	1.79
55	2A	3758	YXM	PAV-CAY	-5.51	1.70	1.79
55	1A	4055	YXM	PAV-CAX	-5.09	1.70	1.79
55	1A	4055	YXM	CAE-NAG	-4.75	1.33	1.45
55	2A	3758	YXM	CAE-NAG	-4.50	1.34	1.45
55	1A	4055	YXM	PAV-CAW	-3.58	1.73	1.79
55	2A	3758	YXM	PAV-CAU	-3.07	1.75	1.80
55	2A	3758	YXM	PAV-CAX	-2.73	1.75	1.79
55	2A	3758	YXM	PAV-CAW	-2.12	1.76	1.79

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	2A	3758	YXM	CAY-PAV-CAX	5.70	120.00	109.26
55	1A	4055	YXM	CAU-PAV-CAW	-4.74	99.65	109.59
55	1A	4055	YXM	CAY-PAV-CAX	4.30	117.35	109.26
55	2A	3758	YXM	CAU-PAV-CAY	-4.20	100.77	109.59
55	2A	3758	YXM	CAU-PAV-CAW	-4.03	101.15	109.59
55	1A	4055	YXM	CAU-PAV-CAY	-4.01	101.19	109.59
55	2A	3758	YXM	CAF-CAE-NAG	3.43	121.96	119.38
55	1A	4055	YXM	CAY-PAV-CAW	2.77	114.48	109.26
55	1A	4055	YXM	CAX-PAV-CAW	2.64	114.23	109.26
55	2A	3758	YXM	PAV-CAU-CAT	-2.54	107.81	114.43
55	2A	3758	YXM	CAU-PAV-CAX	-2.27	104.83	109.59
55	2A	3758	YXM	CAY-PAV-CAW	2.26	113.51	109.26
55	2A	3758	YXM	CAX-PAV-CAW	2.12	113.26	109.26

There are no chirality outliers.

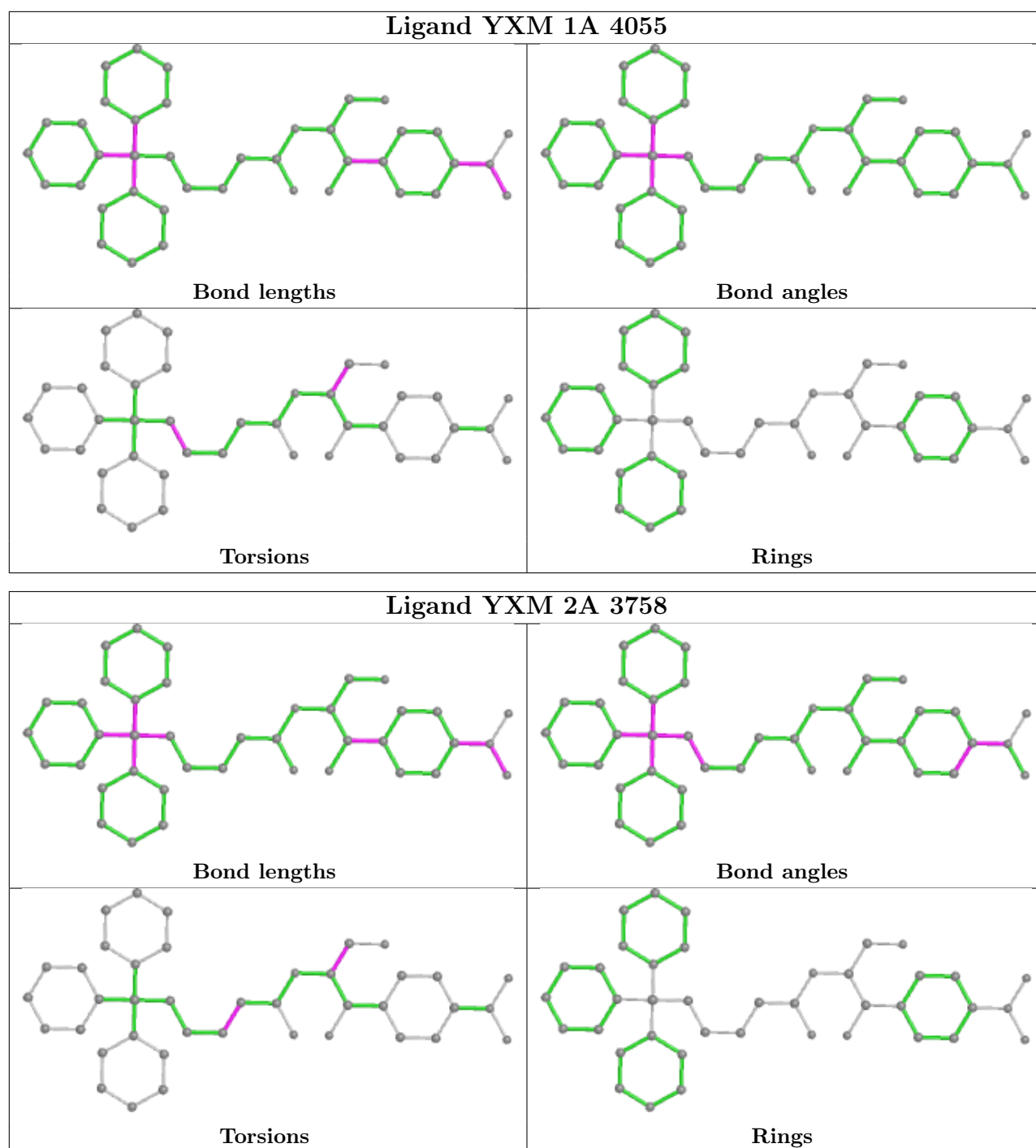
All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	2A	3758	YXM	NAN-CAJ-CAM-OAO
56	1a	3280	MPD	C2-C3-C4-O4
56	2B	220	MPD	C2-C3-C4-C5
57	1F	316	ARG	N-CA-CB-CG
57	1F	316	ARG	C-CA-CB-CG
57	1F	316	ARG	NE-CD-CG-CB
55	2A	3758	YXM	CAH-CAJ-CAM-OAO
57	1F	316	ARG	CA-CB-CG-CD
55	1A	4055	YXM	CAH-CAJ-CAM-OAO
56	2B	220	MPD	O2-C2-C3-C4
55	2A	3758	YXM	CAP-CAR-CAS-CAT
56	18	102	MPD	C2-C3-C4-C5
56	2A	3760	MPD	C2-C3-C4-O4
56	1a	3280	MPD	C1-C2-C3-C4
56	2A	3760	MPD	CM-C2-C3-C4
57	1B	228	ARG	NE-CD-CG-CB
55	1A	4055	YXM	CAS-CAT-CAU-PAV
55	1A	4055	YXM	NAN-CAJ-CAM-OAO
56	1A	4056	MPD	O2-C2-C3-C4
56	2A	3760	MPD	O2-C2-C3-C4
56	1A	4056	MPD	C2-C3-C4-C5
56	2A	3760	MPD	C2-C3-C4-C5
56	18	102	MPD	C2-C3-C4-O4
56	2B	220	MPD	C2-C3-C4-O4

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1A	2861/2915 (98%)	0.53	37 (1%) 77 72	12, 31, 88, 103	0
1	2A	2856/2915 (97%)	0.48	47 (1%) 72 66	25, 50, 91, 104	0
2	1B	120/121 (99%)	0.24	0 100 100	22, 45, 60, 81	0
2	2B	120/121 (99%)	0.34	1 (0%) 86 81	52, 73, 84, 92	0
3	1D	275/276 (99%)	0.36	1 (0%) 92 91	16, 30, 44, 66	0
3	2D	275/276 (99%)	0.64	10 (3%) 42 32	25, 45, 59, 74	0
4	1E	204/206 (99%)	0.25	0 100 100	16, 37, 55, 71	0
4	2E	204/206 (99%)	0.32	2 (0%) 82 77	27, 50, 65, 77	0
5	1F	203/210 (96%)	0.18	0 100 100	15, 36, 59, 73	0
5	2F	203/210 (96%)	0.22	1 (0%) 91 88	27, 60, 73, 83	0
6	1G	181/182 (99%)	0.03	1 (0%) 89 86	39, 59, 72, 82	0
6	2G	181/182 (99%)	1.03	32 (17%) 1 1	68, 78, 84, 88	0
7	1H	174/180 (96%)	0.10	1 (0%) 89 86	36, 49, 62, 66	0
7	2H	173/180 (96%)	0.43	6 (3%) 44 34	61, 75, 82, 87	0
8	1I	147/148 (99%)	0.05	1 (0%) 87 84	38, 66, 77, 80	0
8	2I	146/148 (98%)	-0.02	3 (2%) 63 54	50, 67, 78, 82	0
9	1N	140/140 (100%)	0.24	0 100 100	24, 34, 55, 67	0
9	2N	140/140 (100%)	0.33	1 (0%) 87 84	39, 57, 70, 76	0
10	1O	122/122 (100%)	0.25	0 100 100	22, 35, 50, 59	0
10	2O	122/122 (100%)	0.34	0 100 100	36, 49, 62, 67	0
11	1P	149/150 (99%)	0.21	0 100 100	16, 41, 61, 71	0
11	2P	149/150 (99%)	0.48	5 (3%) 45 35	29, 59, 75, 80	0
12	1Q	141/141 (100%)	0.21	0 100 100	20, 34, 47, 60	0
12	2Q	141/141 (100%)	0.47	3 (2%) 63 54	39, 58, 68, 75	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	0.27	0 100 100	21, 31, 44, 55	0
13	2R	118/118 (100%)	0.39	3 (2%) 57 47	33, 44, 56, 64	0
14	1S	110/112 (98%)	0.03	0 100 100	32, 44, 56, 60	0
14	2S	110/112 (98%)	0.64	8 (7%) 15 8	55, 68, 76, 78	0
15	1T	131/146 (89%)	0.22	1 (0%) 86 81	28, 42, 64, 76	0
15	2T	131/146 (89%)	0.21	0 100 100	39, 51, 69, 74	0
16	1U	116/118 (98%)	0.31	0 100 100	19, 27, 43, 54	0
16	2U	116/118 (98%)	0.43	2 (1%) 70 63	36, 54, 68, 72	0
17	1V	101/101 (100%)	0.17	0 100 100	18, 37, 53, 64	0
17	2V	101/101 (100%)	0.12	0 100 100	35, 63, 73, 76	0
18	1W	112/113 (99%)	0.25	0 100 100	18, 27, 52, 79	0
18	2W	112/113 (99%)	0.38	0 100 100	30, 43, 60, 78	0
19	1X	95/96 (98%)	0.21	0 100 100	18, 32, 52, 67	0
19	2X	95/96 (98%)	0.33	1 (1%) 80 75	41, 53, 63, 70	0
20	1Y	107/110 (97%)	0.13	1 (0%) 84 80	31, 44, 64, 70	0
20	2Y	107/110 (97%)	0.51	4 (3%) 41 31	52, 64, 75, 79	0
21	1Z	203/206 (98%)	0.03	0 100 100	32, 51, 65, 75	0
21	2Z	201/206 (97%)	0.32	12 (5%) 21 14	58, 70, 78, 86	0
22	10	77/85 (90%)	0.20	0 100 100	21, 32, 46, 51	0
22	20	77/85 (90%)	0.89	12 (15%) 2 1	38, 56, 66, 70	0
23	11	97/98 (98%)	0.28	1 (1%) 82 77	21, 37, 60, 68	0
23	21	97/98 (98%)	0.67	4 (4%) 37 27	30, 49, 67, 75	0
24	12	70/72 (97%)	0.12	0 100 100	29, 43, 56, 78	0
24	22	70/72 (97%)	0.17	0 100 100	50, 63, 70, 73	0
25	13	59/60 (98%)	0.14	0 100 100	25, 34, 55, 62	0
25	23	59/60 (98%)	0.53	0 100 100	42, 55, 69, 82	0
26	14	69/71 (97%)	-0.03	1 (1%) 75 70	55, 74, 83, 85	0
26	24	69/71 (97%)	1.07	13 (18%) 1 1	74, 85, 92, 99	0
27	15	59/60 (98%)	0.30	0 100 100	17, 31, 53, 61	0
27	25	59/60 (98%)	0.34	1 (1%) 70 63	29, 45, 60, 73	0
28	16	53/54 (98%)	0.04	0 100 100	28, 36, 50, 57	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.38	1 (1%) 66 59	46, 54, 64, 66	0
29	17	48/49 (97%)	0.42	0 100 100	15, 22, 48, 58	0
29	27	48/49 (97%)	0.64	2 (4%) 36 26	25, 34, 61, 69	0
30	18	64/65 (98%)	0.32	0 100 100	22, 29, 38, 53	0
30	28	64/65 (98%)	0.88	4 (6%) 20 12	40, 48, 55, 66	0
31	19	37/37 (100%)	0.28	0 100 100	26, 36, 53, 56	0
31	29	37/37 (100%)	1.29	9 (24%) 0 0	54, 61, 75, 80	0
32	1a	1488/1521 (97%)	0.33	10 (0%) 87 84	30, 63, 88, 104	0
32	2a	1492/1521 (98%)	0.52	48 (3%) 47 37	42, 71, 91, 103	0
33	1b	231/256 (90%)	0.14	5 (2%) 62 52	60, 73, 81, 85	0
33	2b	231/256 (90%)	0.65	25 (10%) 5 3	67, 80, 86, 90	0
34	1c	206/239 (86%)	0.32	11 (5%) 26 17	52, 67, 75, 79	0
34	2c	206/239 (86%)	0.75	31 (15%) 2 1	65, 78, 85, 89	0
35	1d	208/209 (99%)	0.40	7 (3%) 45 35	51, 63, 73, 80	0
35	2d	208/209 (99%)	0.48	9 (4%) 35 25	58, 67, 76, 80	0
36	1e	148/162 (91%)	0.32	1 (0%) 87 84	42, 59, 69, 74	0
36	2e	148/162 (91%)	0.68	20 (13%) 3 1	58, 69, 76, 87	0
37	1f	100/101 (99%)	0.01	0 100 100	49, 59, 69, 72	0
37	2f	100/101 (99%)	0.04	1 (1%) 82 77	55, 65, 72, 79	0
38	1g	155/156 (99%)	0.08	2 (1%) 77 72	58, 66, 73, 81	0
38	2g	155/156 (99%)	0.92	25 (16%) 1 1	69, 76, 82, 89	0
39	1h	137/138 (99%)	0.35	2 (1%) 73 68	51, 61, 69, 74	0
39	2h	137/138 (99%)	0.36	4 (2%) 51 41	61, 71, 76, 81	0
40	1i	127/128 (99%)	0.69	11 (8%) 10 5	56, 71, 79, 82	0
40	2i	126/128 (98%)	1.84	51 (40%) 0 0	70, 80, 85, 90	0
41	1j	97/105 (92%)	0.67	9 (9%) 8 4	54, 72, 82, 84	0
41	2j	96/105 (91%)	1.32	31 (32%) 0 0	69, 81, 86, 88	0
42	1k	114/129 (88%)	0.12	1 (0%) 84 80	37, 57, 69, 71	0
42	2k	114/129 (88%)	0.40	5 (4%) 34 24	55, 68, 74, 78	0
43	1l	121/132 (91%)	0.34	0 100 100	40, 53, 63, 77	0
43	2l	121/132 (91%)	0.53	9 (7%) 14 8	49, 61, 70, 71	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	116/126 (92%)	0.28	6 (5%) 27 18	56, 68, 75, 80	0
44	2m	114/126 (90%)	1.10	23 (20%) 1 0	71, 79, 86, 88	0
45	1n	60/61 (98%)	0.73	6 (10%) 7 4	57, 65, 72, 76	0
45	2n	60/61 (98%)	2.20	30 (50%) 0 0	70, 80, 88, 89	0
46	1o	88/89 (98%)	0.25	1 (1%) 80 75	43, 59, 71, 78	0
46	2o	88/89 (98%)	0.55	6 (6%) 17 10	57, 68, 77, 83	0
47	1p	82/88 (93%)	0.52	2 (2%) 59 49	53, 65, 74, 81	0
47	2p	82/88 (93%)	0.46	1 (1%) 79 73	54, 63, 74, 76	0
48	1q	99/105 (94%)	0.35	1 (1%) 82 77	50, 61, 69, 75	0
48	2q	99/105 (94%)	0.67	6 (6%) 21 13	55, 62, 72, 76	0
49	1r	68/88 (77%)	-0.04	0 100 100	50, 58, 72, 81	0
49	2r	68/88 (77%)	0.38	2 (2%) 51 41	62, 69, 77, 81	0
50	1s	83/93 (89%)	0.01	1 (1%) 79 73	60, 70, 77, 80	0
50	2s	83/93 (89%)	1.55	26 (31%) 0 0	70, 82, 87, 88	0
51	1t	96/106 (90%)	0.43	4 (4%) 36 26	55, 65, 74, 79	0
51	2t	98/106 (92%)	0.51	2 (2%) 65 56	48, 62, 73, 78	0
52	1u	23/27 (85%)	1.37	5 (21%) 0 0	65, 68, 73, 75	0
52	2u	23/27 (85%)	3.06	18 (78%) 0 0	72, 79, 82, 85	0
53	1y	97/113 (85%)	0.58	5 (5%) 27 18	47, 57, 69, 78	0
53	2y	96/113 (84%)	2.31	52 (54%) 0 0	63, 74, 81, 83	0
All	All	20766/21468 (96%)	0.45	747 (3%) 42 32	12, 57, 84, 104	0

All (747) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
52	2u	14	TRP	8.0
40	2i	127	LYS	7.3
6	2G	39	ILE	7.0
45	2n	2	ALA	6.5
53	2y	40	ILE	6.4
41	2j	54	PHE	6.3
44	2m	102	ARG	6.1
40	2i	126	SER	6.1
23	21	2	SER	6.1
40	2i	115	GLY	6.0

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Mol	Chain	Res	Type	RSRZ
1	1A	1087	G	6.0
45	2n	29	ARG	6.0
53	2y	7	SER	5.7
53	2y	8	LYS	5.7
1	1A	1064	C	5.7
40	2i	109	VAL	5.7
40	2i	75	ASP	5.7
6	2G	152	LEU	5.6
38	2g	33	ASP	5.6
52	2u	13	ILE	5.6
40	2i	71	SER	5.3
45	2n	55	GLY	5.3
40	2i	7	THR	5.3
53	2y	9	GLN	5.2
50	2s	34	TRP	5.1
45	2n	61	TRP	5.1
41	2j	64	GLU	5.1
40	2i	114	TYR	5.0
38	2g	154	TYR	5.0
35	1d	2	GLY	5.0
45	2n	42	ILE	4.9
1	2A	2153	G	4.9
26	24	49	PHE	4.9
40	2i	125	TYR	4.8
53	2y	39	ILE	4.8
34	2c	162	GLN	4.7
50	2s	9	VAL	4.7
32	1a	1036	G	4.7
1	1A	1091	G	4.6
53	2y	42	SER	4.6
32	2a	1030(A)	G	4.6
6	2G	3	LEU	4.5
6	2G	90	LEU	4.5
22	20	76	GLY	4.4
41	2j	40	LEU	4.4
52	2u	2	GLY	4.4
40	2i	10	ARG	4.3
34	2c	160	ALA	4.3
45	2n	3	ARG	4.3
40	2i	63	ILE	4.3
44	2m	66	LEU	4.3
41	2j	65	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
34	2c	163	ALA	4.3
53	2y	50	ALA	4.2
44	2m	87	TYR	4.2
29	27	48	LYS	4.2
53	2y	4	ASN	4.2
1	2A	2106	G	4.1
40	1i	75	ASP	4.1
51	2t	10	LEU	4.1
52	2u	5	ASP	4.1
6	2G	92	VAL	4.1
41	2j	62	HIS	4.0
1	2A	2162	G	4.0
34	1c	2	GLY	4.0
40	2i	69	GLY	4.0
53	2y	5	ILE	4.0
33	2b	152	PHE	4.0
31	29	37	GLY	4.0
35	2d	158	ILE	3.9
34	2c	2	GLY	3.9
45	2n	34	TYR	3.9
53	2y	12	ILE	3.9
1	1A	1076	C	3.9
41	2j	45	ARG	3.9
53	2y	38	HIS	3.9
53	1y	95	ARG	3.9
53	2y	58	ASN	3.9
53	2y	41	LEU	3.8
33	2b	132	LYS	3.8
38	2g	78	ARG	3.8
53	2y	51	ASP	3.8
38	2g	156	TRP	3.8
35	1d	157	LEU	3.8
53	2y	79	ASN	3.8
41	2j	75	ILE	3.8
34	2c	188	LEU	3.7
40	2i	124	GLN	3.7
1	1A	1090	U	3.7
52	2u	4	GLY	3.7
1	1A	1089	G	3.7
52	2u	18	TYR	3.7
45	2n	25	VAL	3.7
41	2j	67	THR	3.7

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Mol	Chain	Res	Type	RSRZ
52	2u	6	ARG	3.7
40	2i	88	TYR	3.7
50	2s	31	ILE	3.6
36	2e	20	GLN	3.6
53	2y	3	MET	3.6
41	2j	48	THR	3.6
40	2i	6	GLY	3.6
41	2j	60	ARG	3.6
32	2a	1257	U	3.6
48	2q	98	LEU	3.6
1	1A	2147	G	3.5
36	2e	22	GLY	3.5
1	2A	2107	C	3.5
6	2G	157	ILE	3.5
48	2q	32	TYR	3.5
44	2m	65	LYS	3.5
14	2S	31	SER	3.5
32	2a	1030(B)	C	3.5
40	2i	50	LEU	3.5
53	2y	74	ILE	3.5
45	2n	49	HIS	3.5
1	1A	1077	A	3.5
34	2c	124	ILE	3.5
40	2i	26	VAL	3.5
1	2A	2147	G	3.5
52	2u	10	ARG	3.5
1	1A	1067	A	3.5
1	2A	2169	A	3.5
41	2j	47	PHE	3.5
40	2i	117	HIS	3.4
45	2n	22	THR	3.4
45	2n	35	ARG	3.4
53	2y	10	MET	3.4
44	1m	2	ALA	3.4
36	2e	17	ALA	3.4
53	2y	70	MET	3.4
1	2A	2125	G	3.4
40	2i	5	TYR	3.4
42	2k	98	LEU	3.4
38	2g	9	VAL	3.4
45	2n	31	ARG	3.4
53	2y	59	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
53	2y	77	LEU	3.4
3	2D	276	LYS	3.4
42	2k	123	LYS	3.4
38	2g	2	ALA	3.4
52	2u	8	THR	3.4
23	2l	26	ARG	3.3
34	2c	190	ARG	3.3
53	2y	6	THR	3.3
1	1A	1103	A	3.3
50	2s	84	GLY	3.3
52	2u	11	GLY	3.3
33	2b	99	GLY	3.3
34	2c	4	LYS	3.3
44	2m	6	GLY	3.3
34	2c	196	LEU	3.3
53	2y	49	VAL	3.3
40	2i	92	TYR	3.3
46	2o	87	ILE	3.3
44	1m	56	LEU	3.3
34	2c	201	TYR	3.3
53	2y	65	GLY	3.3
40	2i	106	ALA	3.3
23	2l	34	THR	3.3
26	14	52	THR	3.3
33	2b	97	TRP	3.3
1	2A	2146	C	3.2
52	2u	3	LYS	3.2
50	2s	2	PRO	3.2
32	2a	1202	G	3.2
53	2y	84	GLN	3.2
33	2b	215	LEU	3.2
32	2a	1036	G	3.2
29	27	1	MET	3.2
39	2h	2	LEU	3.2
41	2j	44	VAL	3.2
50	2s	52	TYR	3.2
53	2y	64	SER	3.2
53	2y	92	GLY	3.2
32	2a	1235	U	3.2
41	2j	68	HIS	3.2
44	2m	106	ASN	3.2
26	24	39	CYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	2A	2174	C	3.2
40	2i	119	ALA	3.2
49	2r	85	LEU	3.2
52	2u	12	LYS	3.2
1	2A	1067	A	3.1
46	2o	86	GLY	3.1
3	2D	219	PRO	3.1
50	2s	33	THR	3.1
21	2Z	125	LEU	3.1
52	1u	5	ASP	3.1
34	2c	195	VAL	3.1
1	1A	1176	G	3.1
1	2A	2159	G	3.1
6	2G	34	LEU	3.1
53	2y	87	LYS	3.1
6	2G	136	ARG	3.1
40	2i	123	PRO	3.1
53	2y	91	LYS	3.1
41	2j	46	ARG	3.1
45	2n	7	ILE	3.1
26	24	10	VAL	3.1
53	2y	88	LEU	3.1
6	2G	131	TYR	3.1
44	2m	116	THR	3.1
45	2n	21	TYR	3.1
40	2i	105	ASP	3.0
32	2a	1373	G	3.0
40	2i	76	ALA	3.0
48	2q	71	PHE	3.0
1	2A	2173	A	3.0
38	2g	80	VAL	3.0
53	2y	86	ASN	3.0
34	2c	200	ALA	3.0
33	1b	129	GLU	3.0
32	1a	1001	A	3.0
32	2a	1354	C	3.0
52	2u	17	THR	3.0
7	2H	41	MET	3.0
52	1u	14	TRP	3.0
6	2G	69	ALA	3.0
26	24	27	THR	3.0
41	2j	39	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	1A	1086	A	3.0
3	2D	50	THR	3.0
38	2g	155	ARG	3.0
53	2y	73	ALA	3.0
1	2A	2140	C	3.0
6	2G	29	TRP	3.0
34	2c	155	GLY	3.0
33	2b	163	PHE	3.0
31	29	11	CYS	3.0
6	2G	62	LEU	2.9
22	20	9	SER	2.9
32	2a	973	G	2.9
50	2s	49	ILE	2.9
53	2y	93	GLU	2.9
33	2b	101	MET	2.9
47	1p	17	TYR	2.9
1	2A	1076	C	2.9
6	2G	160	VAL	2.9
40	2i	70	LYS	2.9
22	20	8	GLY	2.9
33	2b	100	GLY	2.9
2	2B	58	A	2.9
41	2j	43	ARG	2.9
53	2y	90	HIS	2.9
1	1A	2106	G	2.9
26	24	45	GLY	2.9
34	2c	149	ALA	2.9
36	2e	12	LEU	2.9
44	1m	24	GLY	2.9
38	2g	153	HIS	2.9
1	2A	1104	C	2.9
32	1a	1030	C	2.9
50	2s	39	THR	2.9
53	2y	45	PRO	2.9
21	2Z	201	LYS	2.9
38	2g	8	GLU	2.9
41	2j	49	VAL	2.9
53	2y	82	GLU	2.9
34	2c	152	ILE	2.9
41	2j	55	LYS	2.9
33	2b	57	PHE	2.9
7	1H	2	SER	2.8

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Mol	Chain	Res	Type	RSRZ
38	2g	27	ILE	2.8
36	2e	84	PHE	2.8
33	2b	214	ILE	2.8
40	2i	47	LEU	2.8
32	2a	1286	A	2.8
40	2i	21	PRO	2.8
1	1A	1102	C	2.8
40	2i	113	LYS	2.8
44	2m	60	VAL	2.8
26	24	46	GLN	2.8
40	1i	7	THR	2.8
53	2y	53	THR	2.8
46	2o	47	LYS	2.8
11	2P	105	LEU	2.8
9	2N	68	GLU	2.8
44	2m	114	ARG	2.8
53	2y	80	LYS	2.8
6	2G	91	ARG	2.8
41	2j	63	PHE	2.8
38	1g	16	LEU	2.8
50	2s	30	LEU	2.8
35	1d	167	GLY	2.8
41	2j	72	VAL	2.8
44	2m	105	THR	2.8
52	2u	22	ARG	2.8
1	2A	1083	U	2.8
32	2a	1001(A)	G	2.8
21	2Z	197	ILE	2.8
40	1i	127	LYS	2.8
6	2G	139	LEU	2.8
1	1A	2107	C	2.8
32	2a	1234	C	2.8
45	2n	41	ARG	2.7
50	2s	10	PHE	2.7
1	1A	2153	G	2.7
6	2G	43	LEU	2.7
20	2Y	45	VAL	2.7
40	2i	73	GLN	2.7
34	1c	160	ALA	2.7
40	2i	36	TYR	2.7
1	1A	1057	A	2.7
36	2e	109	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
12	2Q	100	GLY	2.7
52	2u	15	ARG	2.7
7	2H	43	VAL	2.7
22	20	72	ARG	2.7
36	2e	21	ALA	2.7
3	2D	55	GLY	2.7
50	2s	79	THR	2.7
1	2A	2139	C	2.7
32	2a	978	A	2.7
6	2G	72	ARG	2.7
40	2i	120	ARG	2.7
30	28	2	PRO	2.7
32	2a	1363(A)	A	2.7
36	2e	105	VAL	2.7
40	1i	14	VAL	2.7
42	2k	13	GLN	2.7
26	24	40	HIS	2.7
40	2i	33	PHE	2.7
46	2o	25	THR	2.7
1	1A	2139	C	2.7
5	2F	181	LEU	2.7
21	2Z	155	LEU	2.7
33	2b	136	VAL	2.7
38	2g	6	ARG	2.7
45	2n	6	LEU	2.7
32	1a	1030(A)	G	2.7
34	1c	159	GLY	2.7
38	2g	7	ALA	2.7
40	1i	8	GLY	2.7
50	2s	83	HIS	2.7
40	2i	18	PHE	2.7
48	1q	98	LEU	2.7
21	2Z	199	LYS	2.7
33	1b	188	ALA	2.7
35	1d	3	ARG	2.7
40	2i	9	ARG	2.7
1	1A	1088	A	2.6
6	2G	138	GLN	2.6
8	2I	3	VAL	2.6
22	20	52	GLY	2.6
1	2A	2148	G	2.6
32	2a	951	G	2.6

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Mol	Chain	Res	Type	RSRZ
36	2e	123	LEU	2.6
31	29	12	ASP	2.6
35	2d	2	GLY	2.6
1	1A	2143	C	2.6
6	2G	2	PRO	2.6
53	2y	52	ALA	2.6
1	2A	1509	C	2.6
44	2m	88	ARG	2.6
32	2a	1224	G	2.6
53	1y	93	GLU	2.6
32	1a	1030(B)	C	2.6
36	2e	13	ILE	2.6
6	2G	70	VAL	2.6
45	2n	56	VAL	2.6
45	1n	2	ALA	2.6
32	2a	975	A	2.6
6	2G	101	ILE	2.6
31	29	13	LYS	2.6
40	2i	8	GLY	2.6
45	2n	33	VAL	2.6
12	2Q	104	PHE	2.6
21	2Z	124	ILE	2.6
52	2u	16	GLY	2.6
53	2y	20	VAL	2.6
26	24	7	PRO	2.6
44	2m	76	ALA	2.6
50	2s	77	THR	2.6
1	1A	1080	C	2.6
6	1G	48	GLU	2.5
20	1Y	1	MET	2.5
1	2A	1064	C	2.5
43	2l	18	VAL	2.5
1	2A	2157	G	2.5
23	1l	2	SER	2.5
45	1n	7	ILE	2.5
14	2S	11	LYS	2.5
46	2o	48	LYS	2.5
52	2u	9	ARG	2.5
53	1y	70	MET	2.5
4	2E	150	VAL	2.5
21	2Z	191	VAL	2.5
1	2A	2124	G	2.5

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Mol	Chain	Res	Type	RSRZ
41	2j	38	ILE	2.5
8	2I	35	LEU	2.5
33	2b	79	ASP	2.5
32	2a	1325	C	2.5
41	2j	59	SER	2.5
34	2c	77	ILE	2.5
38	2g	95	ARG	2.5
41	2j	6	ILE	2.5
38	2g	99	LEU	2.5
1	2A	2179	C	2.5
32	1a	63	C	2.5
51	1t	76	ALA	2.5
32	2a	1324	A	2.5
50	2s	72	GLY	2.5
38	2g	42	ILE	2.5
32	2a	1353	G	2.5
33	2b	164	VAL	2.5
44	2m	64	TRP	2.5
36	2e	16	THR	2.5
35	2d	149	ALA	2.5
1	2A	2138	C	2.5
32	1a	1492	A	2.5
50	2s	62	ILE	2.5
33	2b	118	LEU	2.5
1	2A	2144	U	2.5
1	2A	2152	G	2.5
40	2i	110	GLU	2.5
14	2S	5	THR	2.5
50	2s	82	GLY	2.5
36	2e	43	LEU	2.5
53	2y	78	ILE	2.5
1	2A	1046	A	2.5
20	2Y	7	VAL	2.5
53	2y	95	ARG	2.5
40	1i	5	TYR	2.5
1	1A	1075	C	2.5
1	1A	2161	C	2.5
32	2a	1030	C	2.5
41	1j	44	VAL	2.5
36	2e	45	PHE	2.5
11	2P	34	GLY	2.5
40	2i	116	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
50	2s	8	GLY	2.5
1	2A	2116	G	2.5
44	1m	4	ILE	2.5
48	2q	65	ILE	2.5
1	2A	2145	C	2.4
45	1n	29	ARG	2.4
41	1j	54	PHE	2.4
32	2a	532	A	2.4
36	2e	121	LYS	2.4
7	2H	42	ARG	2.4
33	1b	187	LEU	2.4
33	2b	92	TYR	2.4
51	1t	70	SER	2.4
27	25	60	VAL	2.4
33	1b	133	LYS	2.4
34	2c	159	GLY	2.4
4	2E	114	ALA	2.4
34	2c	65	ALA	2.4
1	2A	2176	A	2.4
52	1u	22	ARG	2.4
53	2y	61	LEU	2.4
44	1m	100	GLY	2.4
35	1d	209	ARG	2.4
45	1n	59	ALA	2.4
53	2y	83	ARG	2.4
34	2c	184	TYR	2.4
42	2k	25	TYR	2.4
6	2G	137	GLU	2.4
32	1a	1034	G	2.4
44	2m	75	ALA	2.4
45	2n	59	ALA	2.4
22	20	46	LYS	2.4
31	29	17	ILE	2.4
41	2j	56	HIS	2.4
50	2s	71	LEU	2.4
41	2j	34	VAL	2.4
32	1a	1001(A)	G	2.4
39	1h	133	LEU	2.4
40	2i	79	LEU	2.4
43	2l	7	ILE	2.4
53	2y	34	LEU	2.4
35	2d	4	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
41	2j	27	ALA	2.4
32	2a	879	C	2.4
1	2A	2168	G	2.4
40	2i	66	ARG	2.4
32	2a	1252	A	2.4
32	2a	1492	A	2.4
47	1p	19	ILE	2.4
38	2g	41	ARG	2.4
31	29	30	PRO	2.4
44	1m	87	TYR	2.4
32	2a	1031	G	2.4
1	2A	652(B)	A	2.4
32	2a	1357	A	2.4
11	2P	59	LEU	2.4
14	2S	10	ARG	2.4
38	2g	32	ARG	2.4
32	2a	979	C	2.4
50	2s	69	HIS	2.3
53	2y	11	GLU	2.3
36	2e	133	TYR	2.3
7	2H	24	VAL	2.3
53	2y	62	VAL	2.3
40	2i	83	ARG	2.3
45	2n	12	ARG	2.3
1	2A	2133	G	2.3
41	1j	74	ILE	2.3
33	2b	78	GLN	2.3
53	2y	60	VAL	2.3
21	2Z	83	PRO	2.3
33	2b	44	LEU	2.3
34	1c	5	ILE	2.3
44	2m	90	LEU	2.3
1	1A	2154	G	2.3
11	2P	68	GLN	2.3
35	2d	112	VAL	2.3
38	2g	69	VAL	2.3
1	2A	2143	C	2.3
41	2j	58	ASP	2.3
6	2G	19	LEU	2.3
39	2h	112	LEU	2.3
40	1i	19	LEU	2.3
41	1j	85	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
45	2n	44	LEU	2.3
3	2D	38	LYS	2.3
20	2Y	63	LYS	2.3
32	2a	1236	A	2.3
32	2a	1306	A	2.3
35	1d	179	GLU	2.3
14	2S	37	ALA	2.3
14	2S	40	ILE	2.3
36	2e	23	GLY	2.3
33	2b	165	VAL	2.3
1	2A	2135	A	2.3
41	1j	20	ALA	2.3
33	2b	162	ILE	2.3
41	1j	36	GLY	2.3
6	2G	37	VAL	2.3
6	2G	48	GLU	2.3
45	1n	61	TRP	2.3
1	2A	2118	U	2.3
1	1A	2117	A	2.3
21	2Z	99	TYR	2.3
32	2a	1093	A	2.3
50	2s	3	ARG	2.3
1	2A	2120	G	2.3
44	2m	27	LYS	2.3
1	1A	1026	U	2.3
22	20	77	ARG	2.3
40	2i	90	PRO	2.3
38	2g	25	ALA	2.3
40	1i	106	ALA	2.3
1	1A	1072	C	2.3
1	2A	1075	C	2.3
8	2I	4	ILE	2.3
34	1c	193	TYR	2.3
1	2A	2127	G	2.3
46	2o	46	HIS	2.2
33	2b	200	ILE	2.2
44	2m	50	GLU	2.2
26	24	56	VAL	2.2
49	2r	87	ARG	2.2
32	2a	1364	U	2.2
40	2i	11	LYS	2.2
41	2j	57	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
8	1I	38	LEU	2.2
13	2R	18	LEU	2.2
45	2n	51	GLY	2.2
31	29	24	TYR	2.2
50	2s	80	TYR	2.2
36	2e	55	VAL	2.2
38	2g	10	ARG	2.2
52	2u	24	ARG	2.2
1	1A	1085	A	2.2
45	2n	60	SER	2.2
40	2i	67	GLY	2.2
45	2n	53	LEU	2.2
35	2d	146	ILE	2.2
47	2p	9	PHE	2.2
44	2m	7	VAL	2.2
6	2G	140	ILE	2.2
22	20	69	PHE	2.2
26	24	5	ILE	2.2
1	2A	2151	G	2.2
41	1j	43	ARG	2.2
26	24	16	CYS	2.2
6	2G	15	VAL	2.2
32	2a	1223	C	2.2
32	2a	1315	U	2.2
1	2A	2134	A	2.2
32	2a	968	A	2.2
34	2c	33	LEU	2.2
6	2G	87	PRO	2.2
34	1c	8	ILE	2.2
42	1k	60	ALA	2.2
44	2m	84	ILE	2.2
1	1A	2141	G	2.2
37	2f	90	VAL	2.2
1	1A	888	C	2.2
1	1A	1104	C	2.2
6	2G	35	GLU	2.2
32	2a	1116	C	2.2
43	2l	16	GLU	2.2
45	1n	8	GLU	2.2
3	2D	182	LEU	2.2
3	2D	217	ARG	2.2
14	2S	57	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
39	1h	112	LEU	2.2
40	2i	37	PHE	2.2
32	2a	1014	A	2.2
7	2H	115	VAL	2.2
16	2U	63	VAL	2.2
34	2c	66	VAL	2.2
34	2c	76	VAL	2.2
43	2l	88	GLY	2.2
32	2a	1320	C	2.2
33	2b	173	ALA	2.2
42	2k	121	PRO	2.2
3	1D	275	LYS	2.2
50	2s	78	ARG	2.2
1	2A	2110	G	2.2
36	2e	89	ILE	2.2
38	2g	152	ALA	2.2
53	2y	75	ASN	2.2
38	2g	77	SER	2.2
43	2l	48	PRO	2.2
30	28	24	ALA	2.1
38	2g	28	ASN	2.1
41	2j	96	ILE	2.1
30	28	21	LYS	2.1
45	2n	23	ARG	2.1
22	20	51	VAL	2.1
35	2d	8	VAL	2.1
35	2d	183	GLY	2.1
32	1a	1035	A	2.1
44	2m	107	ALA	2.1
22	20	11	ARG	2.1
34	2c	206	GLU	2.1
41	2j	66	ARG	2.1
1	2A	2154	G	2.1
32	2a	1222	G	2.1
33	2b	71	VAL	2.1
33	2b	181	PHE	2.1
40	2i	102	LEU	2.1
34	1c	182	ILE	2.1
36	1e	132	ALA	2.1
53	2y	97	ALA	2.1
6	2G	142	PRO	2.1
3	2D	51	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
13	2R	13	HIS	2.1
39	2h	19	VAL	2.1
51	2t	11	SER	2.1
32	2a	1231	G	2.1
43	2l	6	THR	2.1
46	1o	69	TYR	2.1
21	2Z	53	ILE	2.1
32	2a	1287	A	2.1
1	1A	2108	C	2.1
33	2b	133	LYS	2.1
40	2i	53	VAL	2.1
50	1s	77	THR	2.1
6	2G	133	LEU	2.1
19	2X	70	LEU	2.1
22	20	21	LEU	2.1
33	2b	70	PHE	2.1
50	2s	36	ARG	2.1
34	2c	44	GLU	2.1
1	1A	1066	U	2.1
40	1i	81	ILE	2.1
23	2l	4	VAL	2.1
30	28	46	ARG	2.1
48	2q	12	SER	2.1
21	2Z	76	LEU	2.1
22	20	75	LEU	2.1
34	1c	10	PHE	2.1
51	1t	18	GLN	2.1
3	2D	247	ALA	2.1
1	2A	2131	G	2.1
32	2a	971	G	2.1
43	2l	14	GLY	2.1
11	2P	71	VAL	2.1
32	2a	983	A	2.1
32	2a	1531	A	2.1
33	1b	229	VAL	2.1
45	2n	54	PRO	2.1
38	2g	103	TRP	2.1
31	29	15	LYS	2.1
34	1c	201	TYR	2.1
35	2d	166	LYS	2.1
36	2e	88	LYS	2.1
53	1y	87	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	1A	2132	U	2.1
41	1j	50	ILE	2.1
44	2m	78	ILE	2.1
45	2n	10	ALA	2.1
34	2c	148	GLY	2.1
34	2c	171	GLY	2.1
44	2m	104	ARG	2.1
52	1u	10	ARG	2.1
41	1j	72	VAL	2.1
34	2c	186	PHE	2.1
51	1t	13	LEU	2.1
31	29	5	ALA	2.1
40	2i	15	ALA	2.1
44	2m	5	ALA	2.1
53	1y	71	TYR	2.1
12	2Q	59	ARG	2.1
34	2c	80	GLY	2.1
34	2c	194	GLY	2.1
38	1g	82	GLY	2.1
45	2n	19	ARG	2.1
6	2G	38	VAL	2.1
20	2Y	1	MET	2.1
40	2i	108	VAL	2.1
1	1A	2119	A	2.0
26	24	47	GLN	2.0
32	2a	1001	A	2.0
32	2a	1102	A	2.0
34	1c	124	ILE	2.0
48	2q	20	THR	2.0
7	2H	35	VAL	2.0
39	2h	118	VAL	2.0
50	2s	44	MET	2.0
1	1A	2115	G	2.0
1	2A	2137	C	2.0
50	2s	35	SER	2.0
40	1i	46	ALA	2.0
40	1i	12	GLU	2.0
45	2n	38	GLY	2.0
3	2D	40	THR	2.0
45	2n	4	LYS	2.0
1	2A	614(A)	U	2.0
16	2U	41	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
34	1c	149	ALA	2.0
32	2a	1092	A	2.0
32	2a	1503	A	2.0
26	24	44	THR	2.0
13	2R	39	PRO	2.0
14	2S	97	ARG	2.0
34	2c	178	LEU	2.0
36	2e	27	ARG	2.0
40	2i	19	LEU	2.0
41	2j	41	PRO	2.0
43	2l	5	PRO	2.0
43	2l	49	ASN	2.0
52	1u	3	LYS	2.0
21	2Z	179	ASP	2.0
53	2y	94	ALA	2.0
1	1A	1078	U	2.0
1	2A	2165	G	2.0
35	1d	73	ARG	2.0
15	1T	114	LEU	2.0
28	26	11	LEU	2.0
34	2c	175	LEU	2.0
40	2i	85	LEU	2.0
53	2y	37	PRO	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
32	2MG	2a	1207	24/25	0.88	0.22	80,85,90,95	0
1	5MU	2A	1915	21/22	0.89	0.15	74,82,85,99	0
43	0TD	2l	92	10/11	0.90	0.20	52,59,64,79	0
43	0TD	1l	92	10/11	0.91	0.21	43,54,57,67	0
1	PSU	2A	1917	20/21	0.91	0.13	67,77,94,97	0
1	PSU	2A	1911	20/21	0.92	0.13	64,70,80,82	0
1	5MU	1A	1915	21/22	0.93	0.15	64,70,80,81	0
32	M2G	2a	966	25/26	0.93	0.23	64,73,81,89	0
32	5MC	2a	967	21/22	0.93	0.27	71,75,79,86	0
1	PSU	1A	1917	20/21	0.93	0.18	59,64,70,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	4OC	2a	1402	22/23	0.93	0.23	53,63,68,75	0
32	5MC	2a	1404	21/22	0.93	0.23	59,64,70,78	0
32	2MG	1a	1207	24/25	0.93	0.17	60,70,74,76	0
32	7MG	2a	527	24/25	0.94	0.20	53,61,67,69	0
32	PSU	1a	516	20/21	0.95	0.18	51,60,64,64	0
1	4OC	2A	1920	21/23	0.95	0.18	58,66,69,71	0
32	5MC	2a	1400	21/22	0.95	0.30	66,71,75,80	0
32	PSU	2a	516	20/21	0.95	0.14	71,75,83,83	0
32	M2G	1a	966	25/26	0.95	0.24	51,56,62,65	0
32	MA6	2a	1518	24/25	0.95	0.25	53,63,66,68	0
1	PSU	1A	1911	20/21	0.95	0.15	50,59,63,64	0
32	5MC	1a	967	21/22	0.96	0.22	55,62,70,73	0
1	PSU	2A	2605	20/21	0.96	0.24	28,33,39,44	0
32	MA6	2a	1519	24/25	0.96	0.28	54,60,64,66	0
32	7MG	1a	527	24/25	0.96	0.21	39,47,53,55	0
32	MA6	1a	1519	24/25	0.97	0.24	35,41,48,53	0
1	5MC	1A	1962	21/22	0.97	0.21	27,33,36,40	0
1	4OC	1A	1920	21/23	0.97	0.25	35,54,58,62	0
32	4OC	1a	1402	22/23	0.97	0.21	40,46,48,58	0
32	5MC	1a	1404	21/22	0.97	0.21	39,42,49,50	0
32	5MC	1a	1407	21/22	0.97	0.26	34,42,49,50	0
1	5MC	2A	1942	21/22	0.97	0.21	41,48,53,59	0
1	5MC	2A	1962	21/22	0.97	0.20	36,40,49,56	0
32	5MC	2a	1407	21/22	0.97	0.17	54,62,65,77	0
32	UR3	2a	1498	21/22	0.97	0.22	54,58,66,67	0
1	OMG	2A	2251	24/25	0.97	0.22	28,34,39,40	0
1	2MU	2A	2552	21/23	0.97	0.20	28,33,36,40	0
32	MA6	1a	1518	24/25	0.97	0.29	33,40,46,51	0
1	5MU	2A	1939	21/22	0.98	0.20	28,34,36,37	0
32	UR3	1a	1498	21/22	0.98	0.22	36,42,45,55	0
1	OMG	1A	2251	24/25	0.98	0.23	14,19,20,20	0
1	2MA	1A	2503	23/24	0.98	0.22	11,15,18,19	0
1	2MA	2A	2503	23/24	0.98	0.22	24,29,34,35	0
1	2MU	1A	2552	21/23	0.98	0.21	24,27,31,32	0
32	5MC	1a	1400	21/22	0.98	0.23	34,48,52,54	0
1	PSU	1A	2605	20/21	0.98	0.21	20,25,28,30	0
1	5MC	1A	1942	21/22	0.98	0.19	24,30,34,37	0
1	5MU	1A	1939	21/22	0.98	0.21	17,23,25,27	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
54	MG	2a	3025	1/1	0.21	0.25	74,74,74,74	0
54	MG	2a	3195	1/1	0.26	0.13	71,71,71,71	0
58	ZN	14	102	1/1	0.38	0.13	139,139,139,139	0
54	MG	2a	3096	1/1	0.41	0.38	71,71,71,71	0
54	MG	1a	3219	1/1	0.43	0.22	70,70,70,70	0
54	MG	2A	3691	1/1	0.43	0.12	63,63,63,63	0
54	MG	2A	3566	1/1	0.47	0.34	84,84,84,84	0
54	MG	1P	203	1/1	0.47	1.14	49,49,49,49	0
54	MG	1A	3448	1/1	0.47	0.20	28,28,28,28	0
54	MG	1A	3308	1/1	0.52	0.11	82,82,82,82	0
54	MG	2A	3458	1/1	0.53	0.15	55,55,55,55	0
54	MG	2A	3265	1/1	0.55	0.22	66,66,66,66	0
54	MG	2a	3061	1/1	0.56	0.15	75,75,75,75	0
54	MG	2A	3290	1/1	0.56	0.15	36,36,36,36	0
54	MG	1B	210	1/1	0.57	0.11	49,49,49,49	0
58	ZN	24	501	1/1	0.58	0.25	156,156,156,156	0
54	MG	2A	3646	1/1	0.59	0.43	76,76,76,76	0
54	MG	1A	3814	1/1	0.59	0.12	36,36,36,36	0
54	MG	1A	3698	1/1	0.59	0.10	76,76,76,76	0
54	MG	1B	225	1/1	0.59	0.19	53,53,53,53	0
54	MG	2A	3449	1/1	0.60	0.38	64,64,64,64	0
54	MG	1A	3754	1/1	0.60	0.15	49,49,49,49	0
54	MG	2a	3188	1/1	0.60	0.09	77,77,77,77	0
54	MG	2A	3734	1/1	0.61	0.22	67,67,67,67	0
54	MG	1A	3875	1/1	0.61	0.19	47,47,47,47	0
54	MG	2a	3091	1/1	0.62	0.18	59,59,59,59	0
54	MG	2A	3548	1/1	0.64	0.12	34,34,34,34	0
54	MG	2a	3133	1/1	0.64	0.19	60,60,60,60	0
54	MG	1a	3022	1/1	0.64	0.16	59,59,59,59	0
54	MG	1g	202	1/1	0.65	0.33	78,78,78,78	0
54	MG	2A	3716	1/1	0.65	0.20	61,61,61,61	0
54	MG	1y	201	1/1	0.65	0.27	62,62,62,62	0
54	MG	1A	3593	1/1	0.65	0.16	22,22,22,22	0
54	MG	2a	3165	1/1	0.66	0.33	76,76,76,76	0
54	MG	2a	3087	1/1	0.66	0.16	57,57,57,57	0
54	MG	2A	3524	1/1	0.66	0.20	43,43,43,43	0
54	MG	1A	3673	1/1	0.66	0.12	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3074	1/1	0.66	0.50	51,51,51,51	0
54	MG	1a	3040	1/1	0.67	0.30	68,68,68,68	0
54	MG	1A	3781	1/1	0.67	0.17	22,22,22,22	0
54	MG	1A	3988	1/1	0.67	0.11	57,57,57,57	0
54	MG	1A	3887	1/1	0.68	0.09	61,61,61,61	0
54	MG	1a	3187	1/1	0.68	0.10	71,71,71,71	0
54	MG	1A	4015	1/1	0.68	0.79	47,47,47,47	0
54	MG	2A	3456	1/1	0.68	0.31	62,62,62,62	0
54	MG	2A	3205	1/1	0.68	0.38	56,56,56,56	0
54	MG	2A	3488	1/1	0.68	0.56	65,65,65,65	0
54	MG	2a	3119	1/1	0.69	0.33	61,61,61,61	0
54	MG	1a	3082	1/1	0.69	0.24	63,63,63,63	0
54	MG	2a	3161	1/1	0.69	0.10	66,66,66,66	0
54	MG	1A	3289	1/1	0.69	0.19	64,64,64,64	0
54	MG	2a	3174	1/1	0.69	0.11	59,59,59,59	0
54	MG	2a	3180	1/1	0.69	0.08	58,58,58,58	0
54	MG	2a	3184	1/1	0.69	0.10	58,58,58,58	0
54	MG	2A	3398	1/1	0.69	0.15	56,56,56,56	0
54	MG	2A	3686	1/1	0.69	0.10	64,64,64,64	0
54	MG	2A	3509	1/1	0.69	0.12	51,51,51,51	0
54	MG	1n	102	1/1	0.69	0.12	49,49,49,49	0
54	MG	1a	3027	1/1	0.70	0.16	64,64,64,64	0
54	MG	1A	3984	1/1	0.70	0.16	51,51,51,51	0
54	MG	1a	3224	1/1	0.70	0.18	64,64,64,64	0
54	MG	1A	4040	1/1	0.70	0.09	55,55,55,55	0
54	MG	2A	3658	1/1	0.70	0.07	58,58,58,58	0
54	MG	2A	3289	1/1	0.71	0.14	75,75,75,75	0
54	MG	1A	3936	1/1	0.71	0.19	30,30,30,30	0
54	MG	2A	3598	1/1	0.71	0.09	57,57,57,57	0
54	MG	2A	3635	1/1	0.71	0.19	40,40,40,40	0
54	MG	2A	3394	1/1	0.71	0.27	47,47,47,47	0
54	MG	1a	3092	1/1	0.71	0.20	50,50,50,50	0
54	MG	1A	3953	1/1	0.71	0.13	52,52,52,52	0
54	MG	2A	3064	1/1	0.71	0.20	69,69,69,69	0
54	MG	1A	3697	1/1	0.71	0.10	64,64,64,64	0
54	MG	1a	3065	1/1	0.71	0.16	60,60,60,60	0
54	MG	2A	3736	1/1	0.71	0.40	65,65,65,65	0
54	MG	2a	3021	1/1	0.71	0.09	60,60,60,60	0
54	MG	1a	3276	1/1	0.71	0.15	68,68,68,68	0
54	MG	2A	3279	1/1	0.71	0.35	71,71,71,71	0
54	MG	2B	213	1/1	0.72	0.10	77,77,77,77	0
54	MG	1A	3725	1/1	0.72	0.27	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3726	1/1	0.72	0.17	55,55,55,55	0
54	MG	1A	3752	1/1	0.73	0.29	53,53,53,53	0
54	MG	1A	3642	1/1	0.73	0.20	55,55,55,55	0
54	MG	1a	3029	1/1	0.73	0.27	59,59,59,59	0
54	MG	2A	3665	1/1	0.73	0.12	42,42,42,42	0
54	MG	1a	3212	1/1	0.73	0.07	60,60,60,60	0
54	MG	2A	3355	1/1	0.73	0.14	28,28,28,28	0
54	MG	1A	3922	1/1	0.73	0.20	19,19,19,19	0
54	MG	19	103	1/1	0.73	0.44	82,82,82,82	0
54	MG	2a	3103	1/1	0.73	0.20	67,67,67,67	0
54	MG	1a	3240	1/1	0.73	0.37	70,70,70,70	0
54	MG	1A	3034	1/1	0.74	0.23	57,57,57,57	0
54	MG	2A	3605	1/1	0.74	0.08	55,55,55,55	0
54	MG	2A	3625	1/1	0.74	0.12	53,53,53,53	0
54	MG	1a	3249	1/1	0.74	0.11	74,74,74,74	0
54	MG	1a	3199	1/1	0.74	0.08	66,66,66,66	0
54	MG	1A	3658	1/1	0.74	0.16	56,56,56,56	0
54	MG	1A	3321	1/1	0.74	0.13	63,63,63,63	0
54	MG	1a	3165	1/1	0.74	0.39	59,59,59,59	0
54	MG	1A	4051	1/1	0.75	0.29	38,38,38,38	0
54	MG	2a	3168	1/1	0.75	0.14	49,49,49,49	0
54	MG	1A	3694	1/1	0.75	0.12	59,59,59,59	0
54	MG	1A	3878	1/1	0.75	0.15	41,41,41,41	0
54	MG	2A	3257	1/1	0.75	0.30	54,54,54,54	0
54	MG	1A	3405	1/1	0.75	0.11	36,36,36,36	0
54	MG	2V	201	1/1	0.75	0.55	70,70,70,70	0
57	ARG	1F	316	12/12	0.75	0.26	54,60,69,71	0
54	MG	1A	3533	1/1	0.75	0.18	19,19,19,19	0
54	MG	1A	3433	1/1	0.75	0.20	19,19,19,19	0
54	MG	2A	3009	1/1	0.76	0.15	36,36,36,36	0
54	MG	2a	3122	1/1	0.76	0.23	67,67,67,67	0
54	MG	1a	3062	1/1	0.76	0.15	71,71,71,71	0
54	MG	2a	3146	1/1	0.76	0.06	70,70,70,70	0
54	MG	2G	201	1/1	0.76	0.30	78,78,78,78	0
54	MG	2Q	203	1/1	0.76	0.10	51,51,51,51	0
54	MG	1A	3999	1/1	0.76	0.09	55,55,55,55	0
54	MG	2A	3560	1/1	0.76	0.09	66,66,66,66	0
54	MG	2A	3565	1/1	0.76	0.17	60,60,60,60	0
54	MG	1A	3343	1/1	0.76	0.21	22,22,22,22	0
54	MG	2a	3074	1/1	0.76	0.12	66,66,66,66	0
54	MG	2A	3577	1/1	0.76	0.18	30,30,30,30	0
54	MG	2j	201	1/1	0.76	0.13	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3968	1/1	0.76	0.12	25,25,25,25	0
54	MG	2A	3381	1/1	0.76	0.22	58,58,58,58	0
54	MG	2A	3622	1/1	0.76	0.20	66,66,66,66	0
54	MG	2A	3127	1/1	0.77	0.14	60,60,60,60	0
54	MG	2A	3195	1/1	0.77	0.23	66,66,66,66	0
54	MG	1A	3973	1/1	0.77	0.09	50,50,50,50	0
54	MG	2A	3242	1/1	0.77	0.17	66,66,66,66	0
54	MG	1G	201	1/1	0.77	0.20	70,70,70,70	0
54	MG	1A	3728	1/1	0.77	0.09	33,33,33,33	0
54	MG	1d	305	1/1	0.77	0.08	82,82,82,82	0
54	MG	1A	3739	1/1	0.77	0.12	40,40,40,40	0
54	MG	1A	3041	1/1	0.77	0.13	57,57,57,57	0
54	MG	2A	3341	1/1	0.77	0.12	36,36,36,36	0
54	MG	2E	304	1/1	0.77	0.19	26,26,26,26	0
54	MG	2F	301	1/1	0.77	0.19	40,40,40,40	0
54	MG	1A	3406	1/1	0.77	0.16	39,39,39,39	0
54	MG	2P	202	1/1	0.77	0.10	48,48,48,48	0
54	MG	1A	3766	1/1	0.77	0.17	20,20,20,20	0
54	MG	1A	3493	1/1	0.77	0.18	14,14,14,14	0
54	MG	2X	101	1/1	0.77	0.17	59,59,59,59	0
54	MG	2X	102	1/1	0.77	0.14	58,58,58,58	0
54	MG	1A	3412	1/1	0.77	0.15	40,40,40,40	0
54	MG	2A	3435	1/1	0.77	0.46	65,65,65,65	0
54	MG	2A	3445	1/1	0.77	0.11	58,58,58,58	0
54	MG	2A	3186	1/1	0.78	0.17	57,57,57,57	0
54	MG	2A	3519	1/1	0.78	0.57	55,55,55,55	0
54	MG	1A	4003	1/1	0.78	0.24	31,31,31,31	0
54	MG	2G	203	1/1	0.78	0.08	72,72,72,72	0
54	MG	2a	3129	1/1	0.78	0.29	79,79,79,79	0
54	MG	2O	202	1/1	0.78	0.28	63,63,63,63	0
54	MG	1A	3501	1/1	0.78	0.18	29,29,29,29	0
54	MG	2Q	202	1/1	0.78	0.58	44,44,44,44	0
54	MG	1A	3976	1/1	0.78	0.15	61,61,61,61	0
54	MG	1A	3946	1/1	0.78	0.11	45,45,45,45	0
54	MG	1A	3097	1/1	0.78	0.14	49,49,49,49	0
54	MG	1a	3118	1/1	0.78	0.17	55,55,55,55	0
54	MG	2a	3011	1/1	0.78	0.46	73,73,73,73	0
54	MG	2A	3581	1/1	0.78	0.19	36,36,36,36	0
54	MG	2A	3733	1/1	0.78	0.20	82,82,82,82	0
54	MG	1A	3275	1/1	0.78	0.32	49,49,49,49	0
54	MG	1a	3182	1/1	0.78	0.09	52,52,52,52	0
54	MG	2B	211	1/1	0.78	0.21	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3131	1/1	0.78	1.07	61,61,61,61	0
54	MG	1A	3855	1/1	0.79	0.13	39,39,39,39	0
54	MG	2A	3368	1/1	0.79	0.11	63,63,63,63	0
54	MG	2A	3377	1/1	0.79	0.13	63,63,63,63	0
54	MG	2A	3675	1/1	0.79	0.16	49,49,49,49	0
54	MG	1A	3496	1/1	0.79	0.15	22,22,22,22	0
54	MG	2A	3240	1/1	0.79	0.14	65,65,65,65	0
54	MG	1a	3004	1/1	0.79	0.14	58,58,58,58	0
54	MG	2A	3428	1/1	0.79	0.13	81,81,81,81	0
54	MG	1A	3937	1/1	0.79	0.10	39,39,39,39	0
54	MG	1A	3124	1/1	0.79	0.20	50,50,50,50	0
54	MG	2A	3092	1/1	0.79	0.37	66,66,66,66	0
54	MG	2A	3454	1/1	0.79	0.16	42,42,42,42	0
54	MG	1B	217	1/1	0.79	0.15	37,37,37,37	0
54	MG	2D	303	1/1	0.79	0.47	48,48,48,48	0
54	MG	1A	3075	1/1	0.79	0.96	49,49,49,49	0
54	MG	2A	3627	1/1	0.79	0.24	34,34,34,34	0
54	MG	1A	3897	1/1	0.79	0.13	36,36,36,36	0
54	MG	1d	301	1/1	0.80	0.12	54,54,54,54	0
54	MG	1a	3119	1/1	0.80	0.10	49,49,49,49	0
54	MG	1a	3007	1/1	0.80	0.20	55,55,55,55	0
54	MG	2A	3678	1/1	0.80	0.13	29,29,29,29	0
54	MG	2A	3475	1/1	0.80	0.30	57,57,57,57	0
54	MG	2A	3264	1/1	0.80	0.19	57,57,57,57	0
54	MG	2A	3494	1/1	0.80	0.15	55,55,55,55	0
54	MG	2A	3724	1/1	0.80	0.14	58,58,58,58	0
54	MG	2a	3099	1/1	0.80	0.14	76,76,76,76	0
54	MG	1n	101	1/1	0.80	0.16	52,52,52,52	0
54	MG	2A	3512	1/1	0.80	0.41	72,72,72,72	0
54	MG	1A	3692	1/1	0.80	0.19	46,46,46,46	0
54	MG	1A	3238	1/1	0.80	0.15	69,69,69,69	0
54	MG	1a	3189	1/1	0.80	0.14	64,64,64,64	0
54	MG	2A	3549	1/1	0.80	0.17	44,44,44,44	0
54	MG	1A	3605	1/1	0.80	0.15	35,35,35,35	0
54	MG	2A	3352	1/1	0.80	0.14	33,33,33,33	0
54	MG	1A	3995	1/1	0.80	0.21	44,44,44,44	0
54	MG	1A	3499	1/1	0.80	0.20	37,37,37,37	0
54	MG	2A	3123	1/1	0.80	0.15	41,41,41,41	0
54	MG	1A	3181	1/1	0.80	0.12	51,51,51,51	0
54	MG	1P	205	1/1	0.80	0.17	59,59,59,59	0
54	MG	2A	3172	1/1	0.80	0.17	53,53,53,53	0
54	MG	1A	3972	1/1	0.80	0.12	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MPD	2B	220	8/8	0.80	0.26	60,65,71,80	0
54	MG	1a	3264	1/1	0.80	0.16	50,50,50,50	0
54	MG	2A	3199	1/1	0.80	0.21	56,56,56,56	0
54	MG	1A	3354	1/1	0.80	0.18	52,52,52,52	0
54	MG	1A	3688	1/1	0.81	0.18	45,45,45,45	0
54	MG	2a	3050	1/1	0.81	0.14	55,55,55,55	0
54	MG	2A	3515	1/1	0.81	0.10	60,60,60,60	0
54	MG	2a	3070	1/1	0.81	0.16	63,63,63,63	0
54	MG	2A	3087	1/1	0.81	0.21	55,55,55,55	0
54	MG	1a	3051	1/1	0.81	0.12	42,42,42,42	0
54	MG	1H	201	1/1	0.81	0.23	62,62,62,62	0
54	MG	2A	3732	1/1	0.81	0.14	61,61,61,61	0
54	MG	1A	3498	1/1	0.81	0.17	37,37,37,37	0
54	MG	2A	3557	1/1	0.81	0.10	52,52,52,52	0
54	MG	1a	3068	1/1	0.81	0.15	64,64,64,64	0
54	MG	1A	3380	1/1	0.81	0.16	31,31,31,31	0
54	MG	2A	3385	1/1	0.81	0.11	70,70,70,70	0
54	MG	1a	3086	1/1	0.81	0.14	47,47,47,47	0
54	MG	1A	3760	1/1	0.81	0.09	62,62,62,62	0
54	MG	1A	3500	1/1	0.81	0.19	28,28,28,28	0
54	MG	2a	3163	1/1	0.81	0.17	70,70,70,70	0
54	MG	2A	3200	1/1	0.81	0.14	50,50,50,50	0
54	MG	1A	3389	1/1	0.81	0.16	36,36,36,36	0
54	MG	2a	3170	1/1	0.81	0.11	74,74,74,74	0
54	MG	1a	3011	1/1	0.81	0.13	73,73,73,73	0
54	MG	1a	3013	1/1	0.81	0.12	69,69,69,69	0
54	MG	2a	3183	1/1	0.81	0.55	88,88,88,88	0
54	MG	1A	3206	1/1	0.81	0.21	32,32,32,32	0
54	MG	1A	3686	1/1	0.81	0.16	50,50,50,50	0
54	MG	2T	201	1/1	0.81	0.18	63,63,63,63	0
54	MG	2A	3655	1/1	0.81	0.17	52,52,52,52	0
54	MG	2A	3026	1/1	0.81	0.14	43,43,43,43	0
54	MG	2A	3056	1/1	0.81	0.11	64,64,64,64	0
54	MG	2A	3284	1/1	0.81	0.08	45,45,45,45	0
54	MG	1D	310	1/1	0.81	0.35	33,33,33,33	0
54	MG	1A	3982	1/1	0.82	0.28	40,40,40,40	0
54	MG	2A	3247	1/1	0.82	0.45	64,64,64,64	0
54	MG	2A	3460	1/1	0.82	0.15	55,55,55,55	0
54	MG	2A	3050	1/1	0.82	0.62	58,58,58,58	0
54	MG	1A	3930	1/1	0.82	0.27	39,39,39,39	0
54	MG	1A	3484	1/1	0.82	0.14	48,48,48,48	0
54	MG	1A	3751	1/1	0.82	0.13	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3143	1/1	0.82	0.25	57,57,57,57	0
54	MG	1a	3247	1/1	0.82	0.10	62,62,62,62	0
54	MG	2A	3116	1/1	0.82	0.14	61,61,61,61	0
54	MG	2a	3110	1/1	0.82	0.08	54,54,54,54	0
54	MG	2A	3321	1/1	0.82	0.14	57,57,57,57	0
54	MG	1T	201	1/1	0.82	0.24	55,55,55,55	0
54	MG	2A	3343	1/1	0.82	0.11	27,27,27,27	0
54	MG	2a	3132	1/1	0.82	0.32	53,53,53,53	0
54	MG	2A	3346	1/1	0.82	0.15	52,52,52,52	0
54	MG	17	101	1/1	0.82	0.22	37,37,37,37	0
54	MG	2A	3564	1/1	0.82	0.09	55,55,55,55	0
54	MG	1A	3886	1/1	0.82	0.15	33,33,33,33	0
54	MG	1a	3003	1/1	0.82	0.14	61,61,61,61	0
54	MG	1A	3964	1/1	0.82	0.17	68,68,68,68	0
54	MG	1A	3788	1/1	0.82	0.18	37,37,37,37	0
54	MG	2A	3596	1/1	0.82	0.08	51,51,51,51	0
54	MG	1A	3799	1/1	0.82	0.16	32,32,32,32	0
54	MG	1A	3916	1/1	0.82	0.08	56,56,56,56	0
54	MG	1A	3286	1/1	0.82	0.25	56,56,56,56	0
54	MG	2A	3209	1/1	0.82	0.09	49,49,49,49	0
54	MG	2A	3215	1/1	0.82	0.23	60,60,60,60	0
54	MG	2A	3631	1/1	0.82	0.20	74,74,74,74	0
54	MG	2A	3220	1/1	0.82	0.15	54,54,54,54	0
54	MG	28	101	1/1	0.82	0.08	54,54,54,54	0
54	MG	2A	3235	1/1	0.82	0.59	50,50,50,50	0
54	MG	1A	3978	1/1	0.82	0.16	53,53,53,53	0
54	MG	1B	226	1/1	0.83	0.13	60,60,60,60	0
54	MG	2a	3004	1/1	0.83	0.20	41,41,41,41	0
54	MG	2A	3474	1/1	0.83	0.19	60,60,60,60	0
54	MG	2A	3001	1/1	0.83	0.14	51,51,51,51	0
54	MG	2a	3024	1/1	0.83	0.13	43,43,43,43	0
54	MG	1A	3794	1/1	0.83	0.14	19,19,19,19	0
54	MG	2A	3322	1/1	0.83	0.16	38,38,38,38	0
54	MG	2A	3666	1/1	0.83	0.11	54,54,54,54	0
54	MG	2a	3065	1/1	0.83	0.12	58,58,58,58	0
54	MG	2A	3669	1/1	0.83	0.09	44,44,44,44	0
54	MG	2A	3335	1/1	0.83	0.10	38,38,38,38	0
54	MG	1A	3632	1/1	0.83	0.19	52,52,52,52	0
54	MG	2a	3089	1/1	0.83	0.27	71,71,71,71	0
54	MG	2A	3202	1/1	0.83	0.13	40,40,40,40	0
54	MG	1A	3363	1/1	0.83	0.21	17,17,17,17	0
54	MG	2a	3097	1/1	0.83	0.12	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2a	3098	1/1	0.83	0.20	62,62,62,62	0
54	MG	2A	3208	1/1	0.83	0.16	70,70,70,70	0
54	MG	2A	3529	1/1	0.83	0.83	45,45,45,45	0
54	MG	2A	3530	1/1	0.83	1.04	62,62,62,62	0
54	MG	1A	3569	1/1	0.83	0.47	34,34,34,34	0
54	MG	2A	3357	1/1	0.83	0.14	30,30,30,30	0
54	MG	1a	3019	1/1	0.83	0.15	52,52,52,52	0
54	MG	2A	3558	1/1	0.83	0.13	56,56,56,56	0
54	MG	2A	3753	1/1	0.83	0.11	57,57,57,57	0
54	MG	1A	3871	1/1	0.83	0.18	19,19,19,19	0
54	MG	2A	3227	1/1	0.83	0.11	52,52,52,52	0
54	MG	2A	3080	1/1	0.83	1.21	57,57,57,57	0
54	MG	2D	309	1/1	0.83	0.20	58,58,58,58	0
54	MG	2D	311	1/1	0.83	0.13	33,33,33,33	0
54	MG	1A	3148	1/1	0.83	0.11	50,50,50,50	0
54	MG	1B	224	1/1	0.83	0.16	64,64,64,64	0
54	MG	2A	3400	1/1	0.83	0.09	46,46,46,46	0
54	MG	2A	3246	1/1	0.83	0.14	51,51,51,51	0
54	MG	1a	3122	1/1	0.83	0.51	75,75,75,75	0
54	MG	1a	3032	1/1	0.83	0.33	58,58,58,58	0
54	MG	2A	3607	1/1	0.83	0.14	56,56,56,56	0
54	MG	2A	3620	1/1	0.83	0.15	28,28,28,28	0
54	MG	1a	3034	1/1	0.83	0.12	47,47,47,47	0
54	MG	1A	3414	1/1	0.83	0.19	15,15,15,15	0
54	MG	2A	3168	1/1	0.83	0.12	54,54,54,54	0
54	MG	1a	3042	1/1	0.83	0.27	62,62,62,62	0
54	MG	2A	3018	1/1	0.84	0.13	36,36,36,36	0
54	MG	2A	3690	1/1	0.84	0.07	59,59,59,59	0
54	MG	2a	3055	1/1	0.84	0.12	68,68,68,68	0
54	MG	2A	3537	1/1	0.84	0.50	65,65,65,65	0
54	MG	1A	3191	1/1	0.84	0.34	45,45,45,45	0
54	MG	1A	3304	1/1	0.84	0.16	39,39,39,39	0
54	MG	2A	3725	1/1	0.84	0.12	59,59,59,59	0
54	MG	1Z	301	1/1	0.84	0.23	62,62,62,62	0
54	MG	2A	3058	1/1	0.84	0.13	60,60,60,60	0
54	MG	1a	3201	1/1	0.84	0.13	73,73,73,73	0
54	MG	1a	3204	1/1	0.84	0.15	47,47,47,47	0
54	MG	1A	3706	1/1	0.84	0.20	62,62,62,62	0
54	MG	2A	3743	1/1	0.84	0.17	54,54,54,54	0
54	MG	1a	3052	1/1	0.84	0.14	57,57,57,57	0
54	MG	2A	3755	1/1	0.84	0.13	50,50,50,50	0
54	MG	2A	3574	1/1	0.84	0.12	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1a	3057	1/1	0.84	0.12	75,75,75,75	0
54	MG	2A	3448	1/1	0.84	0.10	46,46,46,46	0
54	MG	1A	3539	1/1	0.84	0.14	55,55,55,55	0
54	MG	1A	3171	1/1	0.84	0.19	47,47,47,47	0
54	MG	1A	3476	1/1	0.84	0.24	12,12,12,12	0
54	MG	2a	3144	1/1	0.84	0.10	62,62,62,62	0
54	MG	1A	3803	1/1	0.84	0.15	39,39,39,39	0
54	MG	2A	3150	1/1	0.84	0.80	66,66,66,66	0
54	MG	2G	202	1/1	0.84	0.08	67,67,67,67	0
54	MG	2A	3463	1/1	0.84	0.20	64,64,64,64	0
54	MG	2A	3167	1/1	0.84	0.31	56,56,56,56	0
54	MG	1A	3813	1/1	0.84	0.08	69,69,69,69	0
54	MG	1A	3594	1/1	0.84	0.12	31,31,31,31	0
54	MG	2A	3491	1/1	0.84	0.22	63,63,63,63	0
54	MG	2A	3492	1/1	0.84	0.20	23,23,23,23	0
54	MG	1F	313	1/1	0.84	0.37	58,58,58,58	0
54	MG	1A	3217	1/1	0.84	0.24	57,57,57,57	0
54	MG	2a	3191	1/1	0.84	0.15	75,75,75,75	0
54	MG	1A	3859	1/1	0.84	0.17	14,14,14,14	0
54	MG	2e	202	1/1	0.84	0.06	66,66,66,66	0
54	MG	1a	3135	1/1	0.84	0.13	41,41,41,41	0
56	MPD	2A	3760	8/8	0.84	0.30	54,60,63,69	0
54	MG	1a	3162	1/1	0.84	0.37	64,64,64,64	0
54	MG	1N	204	1/1	0.84	0.09	47,47,47,47	0
54	MG	1A	3615	1/1	0.84	0.12	52,52,52,52	0
54	MG	2A	3685	1/1	0.84	0.11	50,50,50,50	0
54	MG	1A	3102	1/1	0.85	0.10	48,48,48,48	0
54	MG	1A	3598	1/1	0.85	0.58	34,34,34,34	0
54	MG	1A	3604	1/1	0.85	0.20	25,25,25,25	0
54	MG	2A	3362	1/1	0.85	0.13	30,30,30,30	0
54	MG	2A	3148	1/1	0.85	0.47	46,46,46,46	0
54	MG	2a	3006	1/1	0.85	0.15	67,67,67,67	0
54	MG	1A	3220	1/1	0.85	0.59	34,34,34,34	0
54	MG	2a	3014	1/1	0.85	0.13	71,71,71,71	0
54	MG	2A	3154	1/1	0.85	0.68	64,64,64,64	0
54	MG	1A	3861	1/1	0.85	0.11	50,50,50,50	0
54	MG	1a	3233	1/1	0.85	0.14	65,65,65,65	0
54	MG	2a	3033	1/1	0.85	0.13	57,57,57,57	0
54	MG	1A	3159	1/1	0.85	0.35	33,33,33,33	0
54	MG	2a	3051	1/1	0.85	0.20	79,79,79,79	0
54	MG	2A	3636	1/1	0.85	0.18	57,57,57,57	0
54	MG	1a	3242	1/1	0.85	0.18	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3193	1/1	0.85	0.38	59,59,59,59	0
54	MG	2a	3069	1/1	0.85	0.19	74,74,74,74	0
54	MG	1F	315	1/1	0.85	0.29	60,60,60,60	0
54	MG	2A	3441	1/1	0.85	0.29	51,51,51,51	0
54	MG	2a	3076	1/1	0.85	0.13	68,68,68,68	0
54	MG	1A	3239	1/1	0.85	0.32	56,56,56,56	0
54	MG	1a	3053	1/1	0.85	0.14	61,61,61,61	0
54	MG	1A	3266	1/1	0.85	0.14	62,62,62,62	0
54	MG	1A	3415	1/1	0.85	0.18	19,19,19,19	0
54	MG	1A	3349	1/1	0.85	0.20	14,14,14,14	0
54	MG	1A	3680	1/1	0.85	0.19	63,63,63,63	0
54	MG	2A	3214	1/1	0.85	0.16	45,45,45,45	0
54	MG	1a	3072	1/1	0.85	0.10	64,64,64,64	0
54	MG	1A	3270	1/1	0.85	0.14	47,47,47,47	0
54	MG	2A	3224	1/1	0.85	0.12	48,48,48,48	0
54	MG	1A	4000	1/1	0.85	0.13	67,67,67,67	0
54	MG	2A	3230	1/1	0.85	0.51	59,59,59,59	0
54	MG	1y	202	1/1	0.85	0.18	53,53,53,53	0
54	MG	1A	3551	1/1	0.85	0.13	48,48,48,48	0
54	MG	2A	3241	1/1	0.85	0.11	53,53,53,53	0
54	MG	1a	3104	1/1	0.85	0.18	61,61,61,61	0
54	MG	1A	4004	1/1	0.85	0.14	36,36,36,36	0
54	MG	1a	3001	1/1	0.85	0.17	77,77,77,77	0
54	MG	2A	3045	1/1	0.85	0.12	45,45,45,45	0
54	MG	2B	205	1/1	0.85	0.15	59,59,59,59	0
54	MG	2A	3262	1/1	0.85	0.14	50,50,50,50	0
54	MG	1a	3002	1/1	0.85	0.11	61,61,61,61	0
54	MG	1A	4013	1/1	0.85	0.17	27,27,27,27	0
54	MG	1a	3143	1/1	0.85	0.14	49,49,49,49	0
54	MG	1A	3200	1/1	0.85	0.44	47,47,47,47	0
54	MG	2A	3065	1/1	0.85	0.21	41,41,41,41	0
54	MG	1A	4024	1/1	0.85	0.14	48,48,48,48	0
54	MG	2a	3194	1/1	0.85	0.14	72,72,72,72	0
54	MG	1A	3795	1/1	0.85	0.35	37,37,37,37	0
54	MG	1A	3592	1/1	0.85	0.08	52,52,52,52	0
54	MG	2A	3332	1/1	0.85	0.14	48,48,48,48	0
54	MG	1A	3109	1/1	0.85	0.50	60,60,60,60	0
54	MG	2A	3097	1/1	0.85	0.15	44,44,44,44	0
54	MG	2A	3098	1/1	0.85	0.12	47,47,47,47	0
54	MG	1B	213	1/1	0.85	0.10	59,59,59,59	0
54	MG	2A	3582	1/1	0.85	0.07	48,48,48,48	0
54	MG	1a	3179	1/1	0.86	0.10	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3189	1/1	0.86	0.69	44,44,44,44	0
54	MG	2A	3323	1/1	0.86	0.09	55,55,55,55	0
54	MG	1A	3704	1/1	0.86	0.11	52,52,52,52	0
54	MG	1A	3185	1/1	0.86	0.10	52,52,52,52	0
54	MG	2A	3337	1/1	0.86	0.18	21,21,21,21	0
54	MG	1A	3714	1/1	0.86	0.17	50,50,50,50	0
54	MG	2A	3342	1/1	0.86	0.13	35,35,35,35	0
54	MG	1A	3614	1/1	0.86	0.10	46,46,46,46	0
54	MG	1A	3319	1/1	0.86	0.36	63,63,63,63	0
54	MG	2A	3578	1/1	0.86	0.17	32,32,32,32	0
54	MG	1A	4021	1/1	0.86	0.46	43,43,43,43	0
54	MG	1A	4023	1/1	0.86	0.06	85,85,85,85	0
54	MG	1A	3732	1/1	0.86	0.22	38,38,38,38	0
54	MG	1A	4032	1/1	0.86	0.51	58,58,58,58	0
54	MG	2A	3602	1/1	0.86	0.15	38,38,38,38	0
54	MG	2A	3170	1/1	0.86	0.11	59,59,59,59	0
54	MG	2A	3171	1/1	0.86	0.40	50,50,50,50	0
54	MG	2a	3032	1/1	0.86	0.07	66,66,66,66	0
54	MG	1A	3617	1/1	0.86	0.13	36,36,36,36	0
54	MG	1A	3894	1/1	0.86	0.16	31,31,31,31	0
54	MG	2A	3393	1/1	0.86	0.18	44,44,44,44	0
54	MG	1B	202	1/1	0.86	0.18	58,58,58,58	0
54	MG	1A	3741	1/1	0.86	0.19	36,36,36,36	0
54	MG	2A	3634	1/1	0.86	0.16	27,27,27,27	0
54	MG	1A	3377	1/1	0.86	0.13	43,43,43,43	0
54	MG	1a	3268	1/1	0.86	0.09	76,76,76,76	0
54	MG	2a	3072	1/1	0.86	0.12	61,61,61,61	0
54	MG	1A	3248	1/1	0.86	1.16	36,36,36,36	0
54	MG	2A	3654	1/1	0.86	0.10	63,63,63,63	0
54	MG	1A	3645	1/1	0.86	0.16	30,30,30,30	0
54	MG	1A	3534	1/1	0.86	0.26	53,53,53,53	0
54	MG	2A	3446	1/1	0.86	0.07	37,37,37,37	0
54	MG	1A	3384	1/1	0.86	0.15	26,26,26,26	0
54	MG	1l	202	1/1	0.86	0.08	59,59,59,59	0
54	MG	2A	3671	1/1	0.86	0.21	72,72,72,72	0
54	MG	2A	3451	1/1	0.86	0.10	50,50,50,50	0
54	MG	1A	3674	1/1	0.86	0.27	25,25,25,25	0
54	MG	1A	3474	1/1	0.86	0.10	37,37,37,37	0
54	MG	1A	3387	1/1	0.86	0.16	42,42,42,42	0
54	MG	2a	3120	1/1	0.86	0.11	55,55,55,55	0
54	MG	1a	3075	1/1	0.86	0.20	50,50,50,50	0
54	MG	1A	3687	1/1	0.86	0.06	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3695	1/1	0.86	0.13	59,59,59,59	0
54	MG	2A	3468	1/1	0.86	0.11	65,65,65,65	0
54	MG	2A	3718	1/1	0.86	0.15	51,51,51,51	0
54	MG	1A	3335	1/1	0.86	0.11	57,57,57,57	0
54	MG	1A	3801	1/1	0.86	0.10	50,50,50,50	0
54	MG	2A	3477	1/1	0.86	0.14	58,58,58,58	0
54	MG	2A	3481	1/1	0.86	0.17	19,19,19,19	0
54	MG	1A	3491	1/1	0.86	0.22	12,12,12,12	0
54	MG	2A	3036	1/1	0.86	0.27	70,70,70,70	0
54	MG	1a	3113	1/1	0.86	0.13	52,52,52,52	0
54	MG	1A	3807	1/1	0.86	0.12	29,29,29,29	0
54	MG	2a	3181	1/1	0.86	0.11	53,53,53,53	0
54	MG	2A	3502	1/1	0.86	0.18	74,74,74,74	0
54	MG	1A	3393	1/1	0.86	0.15	52,52,52,52	0
54	MG	1A	3223	1/1	0.86	0.28	27,27,27,27	0
54	MG	2B	206	1/1	0.86	0.36	78,78,78,78	0
54	MG	1l	102	1/1	0.86	0.53	48,48,48,48	0
54	MG	2B	212	1/1	0.86	0.15	53,53,53,53	0
54	MG	2a	3197	1/1	0.86	0.11	56,56,56,56	0
54	MG	1A	3825	1/1	0.86	0.46	25,25,25,25	0
54	MG	1a	3151	1/1	0.86	0.25	73,73,73,73	0
54	MG	1A	3844	1/1	0.86	0.11	43,43,43,43	0
54	MG	1A	3997	1/1	0.86	0.13	45,45,45,45	0
54	MG	1a	3178	1/1	0.86	0.18	47,47,47,47	0
54	MG	2A	3539	1/1	0.86	0.13	68,68,68,68	0
54	MG	2A	3544	1/1	0.86	0.24	58,58,58,58	0
54	MG	2A	3274	1/1	0.87	0.46	63,63,63,63	0
54	MG	2A	3462	1/1	0.87	0.13	37,37,37,37	0
54	MG	2A	3633	1/1	0.87	0.07	74,74,74,74	0
54	MG	28	102	1/1	0.87	0.15	52,52,52,52	0
54	MG	1A	3749	1/1	0.87	0.08	50,50,50,50	0
54	MG	2a	3005	1/1	0.87	0.29	50,50,50,50	0
54	MG	2A	3135	1/1	0.87	0.18	72,72,72,72	0
54	MG	2A	3142	1/1	0.87	0.11	58,58,58,58	0
54	MG	1a	3273	1/1	0.87	0.09	72,72,72,72	0
54	MG	1D	316	1/1	0.87	0.42	41,41,41,41	0
54	MG	2A	3479	1/1	0.87	0.14	47,47,47,47	0
54	MG	1A	3820	1/1	0.87	0.09	58,58,58,58	0
54	MG	2A	3662	1/1	0.87	0.06	64,64,64,64	0
54	MG	2A	3664	1/1	0.87	0.13	62,62,62,62	0
54	MG	2a	3039	1/1	0.87	0.13	77,77,77,77	0
54	MG	2a	3041	1/1	0.87	0.13	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3485	1/1	0.87	0.14	62,62,62,62	0
54	MG	1d	304	1/1	0.87	0.14	46,46,46,46	0
54	MG	1A	3607	1/1	0.87	0.18	53,53,53,53	0
54	MG	1A	3939	1/1	0.87	0.08	42,42,42,42	0
54	MG	1A	3691	1/1	0.87	0.10	53,53,53,53	0
54	MG	2A	3496	1/1	0.87	0.08	50,50,50,50	0
54	MG	2A	3680	1/1	0.87	0.08	29,29,29,29	0
54	MG	2A	3500	1/1	0.87	0.25	65,65,65,65	0
54	MG	1a	3037	1/1	0.87	0.15	38,38,38,38	0
54	MG	1A	3152	1/1	0.87	0.13	40,40,40,40	0
54	MG	2a	3077	1/1	0.87	0.10	58,58,58,58	0
54	MG	1a	3168	1/1	0.87	0.13	68,68,68,68	0
54	MG	2A	3194	1/1	0.87	0.35	57,57,57,57	0
54	MG	2A	3709	1/1	0.87	0.60	70,70,70,70	0
54	MG	1A	3459	1/1	0.87	0.10	45,45,45,45	0
54	MG	1a	3047	1/1	0.87	0.12	59,59,59,59	0
54	MG	1A	3472	1/1	0.87	0.12	42,42,42,42	0
54	MG	1R	203	1/1	0.87	0.30	39,39,39,39	0
54	MG	1a	3188	1/1	0.87	0.26	60,60,60,60	0
54	MG	1A	4031	1/1	0.87	0.15	33,33,33,33	0
54	MG	2A	3380	1/1	0.87	0.26	28,28,28,28	0
54	MG	1a	3190	1/1	0.87	0.09	50,50,50,50	0
54	MG	1A	3402	1/1	0.87	0.17	25,25,25,25	0
54	MG	2A	3552	1/1	0.87	0.09	47,47,47,47	0
54	MG	2A	3744	1/1	0.87	0.19	54,54,54,54	0
54	MG	1a	3200	1/1	0.87	0.12	55,55,55,55	0
54	MG	1A	4033	1/1	0.87	0.11	29,29,29,29	0
54	MG	2A	3756	1/1	0.87	0.25	53,53,53,53	0
54	MG	2a	3149	1/1	0.87	0.08	64,64,64,64	0
54	MG	1A	3339	1/1	0.87	0.15	28,28,28,28	0
54	MG	1A	3063	1/1	0.87	0.15	24,24,24,24	0
54	MG	2B	207	1/1	0.87	0.17	63,63,63,63	0
54	MG	2A	3423	1/1	0.87	0.15	69,69,69,69	0
54	MG	1A	3383	1/1	0.87	0.10	28,28,28,28	0
54	MG	2A	3573	1/1	0.87	0.07	59,59,59,59	0
54	MG	2A	3433	1/1	0.87	0.24	39,39,39,39	0
54	MG	2D	304	1/1	0.87	1.57	44,44,44,44	0
54	MG	1A	3108	1/1	0.87	0.73	35,35,35,35	0
54	MG	2A	3436	1/1	0.87	0.18	70,70,70,70	0
54	MG	1A	3074	1/1	0.87	0.13	37,37,37,37	0
54	MG	1A	3419	1/1	0.87	0.14	19,19,19,19	0
54	MG	2A	3584	1/1	0.87	0.21	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3095	1/1	0.87	0.14	60,60,60,60	0
54	MG	1a	3090	1/1	0.87	0.11	50,50,50,50	0
54	MG	2I	201	1/1	0.87	0.09	66,66,66,66	0
54	MG	1A	3902	1/1	0.87	0.16	32,32,32,32	0
54	MG	1A	3421	1/1	0.87	0.24	43,43,43,43	0
54	MG	2A	3452	1/1	0.87	0.09	74,74,74,74	0
54	MG	1a	3253	1/1	0.87	0.07	61,61,61,61	0
54	MG	1A	3359	1/1	0.87	0.14	31,31,31,31	0
54	MG	2A	3130	1/1	0.87	0.11	52,52,52,52	0
54	MG	2B	214	1/1	0.88	0.18	60,60,60,60	0
54	MG	17	103	1/1	0.88	0.67	30,30,30,30	0
54	MG	2A	3536	1/1	0.88	0.11	46,46,46,46	0
54	MG	2A	3059	1/1	0.88	0.19	45,45,45,45	0
54	MG	2A	3286	1/1	0.88	0.24	54,54,54,54	0
54	MG	2E	301	1/1	0.88	0.28	35,35,35,35	0
54	MG	2A	3060	1/1	0.88	0.15	27,27,27,27	0
54	MG	17	104	1/1	0.88	0.19	36,36,36,36	0
54	MG	2A	3306	1/1	0.88	0.13	36,36,36,36	0
54	MG	2A	3309	1/1	0.88	0.10	25,25,25,25	0
54	MG	2A	3554	1/1	0.88	0.07	60,60,60,60	0
54	MG	19	101	1/1	0.88	0.21	57,57,57,57	0
54	MG	1A	3676	1/1	0.88	0.16	14,14,14,14	0
54	MG	1A	3329	1/1	0.88	0.25	69,69,69,69	0
54	MG	2A	3083	1/1	0.88	0.37	39,39,39,39	0
54	MG	1A	3681	1/1	0.88	0.25	25,25,25,25	0
54	MG	2A	3089	1/1	0.88	0.58	43,43,43,43	0
54	MG	1A	3915	1/1	0.88	0.07	39,39,39,39	0
54	MG	1A	3574	1/1	0.88	0.13	34,34,34,34	0
54	MG	1A	3153	1/1	0.88	0.22	33,33,33,33	0
54	MG	1A	3923	1/1	0.88	0.21	32,32,32,32	0
54	MG	1A	4035	1/1	0.88	0.21	43,43,43,43	0
54	MG	1A	3027	1/1	0.88	0.10	64,64,64,64	0
54	MG	1a	3020	1/1	0.88	0.46	61,61,61,61	0
54	MG	2A	3592	1/1	0.88	0.10	30,30,30,30	0
54	MG	2a	3007	1/1	0.88	0.08	62,62,62,62	0
54	MG	1A	3342	1/1	0.88	0.19	54,54,54,54	0
54	MG	1A	3165	1/1	0.88	0.15	49,49,49,49	0
54	MG	2A	3599	1/1	0.88	0.05	45,45,45,45	0
54	MG	2A	3134	1/1	0.88	0.12	47,47,47,47	0
54	MG	1a	3028	1/1	0.88	0.16	49,49,49,49	0
54	MG	2a	3028	1/1	0.88	0.15	71,71,71,71	0
54	MG	2A	3136	1/1	0.88	0.18	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3612	1/1	0.88	0.07	48,48,48,48	0
54	MG	2a	3036	1/1	0.88	0.10	50,50,50,50	0
54	MG	1a	3203	1/1	0.88	0.11	69,69,69,69	0
54	MG	2A	3391	1/1	0.88	0.17	46,46,46,46	0
54	MG	2a	3046	1/1	0.88	0.20	62,62,62,62	0
54	MG	2A	3623	1/1	0.88	0.07	39,39,39,39	0
54	MG	1A	3284	1/1	0.88	0.12	53,53,53,53	0
54	MG	2a	3052	1/1	0.88	0.11	54,54,54,54	0
54	MG	1a	3031	1/1	0.88	0.13	45,45,45,45	0
54	MG	1A	3054	1/1	0.88	0.16	23,23,23,23	0
54	MG	2a	3062	1/1	0.88	0.36	62,62,62,62	0
54	MG	2A	3160	1/1	0.88	0.13	49,49,49,49	0
54	MG	2a	3066	1/1	0.88	0.12	59,59,59,59	0
54	MG	2A	3409	1/1	0.88	0.44	62,62,62,62	0
54	MG	1A	3358	1/1	0.88	0.15	26,26,26,26	0
54	MG	2a	3071	1/1	0.88	0.36	61,61,61,61	0
54	MG	2A	3424	1/1	0.88	0.30	61,61,61,61	0
54	MG	2A	3643	1/1	0.88	0.12	54,54,54,54	0
54	MG	1A	3082	1/1	0.88	0.12	34,34,34,34	0
54	MG	2A	3652	1/1	0.88	0.09	58,58,58,58	0
54	MG	1A	3232	1/1	0.88	0.78	39,39,39,39	0
54	MG	1A	3970	1/1	0.88	0.23	43,43,43,43	0
54	MG	1D	301	1/1	0.88	0.79	28,28,28,28	0
54	MG	2A	3440	1/1	0.88	0.20	50,50,50,50	0
54	MG	1A	3055	1/1	0.88	0.22	45,45,45,45	0
54	MG	2A	3192	1/1	0.88	0.12	73,73,73,73	0
54	MG	1A	3503	1/1	0.88	0.18	15,15,15,15	0
54	MG	1E	304	1/1	0.88	0.16	15,15,15,15	0
54	MG	2a	3104	1/1	0.88	0.09	61,61,61,61	0
54	MG	1A	3634	1/1	0.88	0.09	58,58,58,58	0
54	MG	2a	3118	1/1	0.88	0.09	48,48,48,48	0
54	MG	1a	3270	1/1	0.88	0.14	56,56,56,56	0
54	MG	1a	3271	1/1	0.88	0.12	60,60,60,60	0
54	MG	2a	3121	1/1	0.88	0.10	68,68,68,68	0
54	MG	1A	3852	1/1	0.88	0.25	42,42,42,42	0
54	MG	1A	3636	1/1	0.88	0.19	25,25,25,25	0
54	MG	1A	3737	1/1	0.88	0.17	36,36,36,36	0
54	MG	2A	3687	1/1	0.88	0.22	66,66,66,66	0
54	MG	2a	3138	1/1	0.88	0.45	59,59,59,59	0
54	MG	1d	302	1/1	0.88	0.17	48,48,48,48	0
54	MG	1A	3099	1/1	0.88	0.34	37,37,37,37	0
54	MG	1A	3011	1/1	0.88	0.42	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2a	3152	1/1	0.88	0.13	77,77,77,77	0
54	MG	2a	3158	1/1	0.88	0.10	81,81,81,81	0
54	MG	2A	3702	1/1	0.88	0.23	66,66,66,66	0
54	MG	1A	3873	1/1	0.88	0.13	24,24,24,24	0
54	MG	2A	3222	1/1	0.88	0.11	50,50,50,50	0
54	MG	1a	3083	1/1	0.88	0.15	69,69,69,69	0
54	MG	1A	3743	1/1	0.88	0.17	55,55,55,55	0
54	MG	1R	204	1/1	0.88	0.20	38,38,38,38	0
54	MG	2A	3233	1/1	0.88	0.23	49,49,49,49	0
54	MG	1A	3458	1/1	0.88	0.11	47,47,47,47	0
54	MG	1a	3101	1/1	0.88	0.11	48,48,48,48	0
54	MG	1A	3883	1/1	0.88	0.14	48,48,48,48	0
54	MG	2A	3006	1/1	0.88	0.18	52,52,52,52	0
54	MG	1A	3323	1/1	0.88	0.20	40,40,40,40	0
54	MG	1a	3116	1/1	0.88	0.17	54,54,54,54	0
54	MG	2A	3254	1/1	0.88	0.26	59,59,59,59	0
54	MG	15	103	1/1	0.88	0.57	32,32,32,32	0
54	MG	16	101	1/1	0.88	0.08	39,39,39,39	0
54	MG	1A	3562	1/1	0.88	0.13	22,22,22,22	0
56	MPD	2A	3759	8/8	0.88	0.42	37,46,50,56	0
54	MG	1a	3131	1/1	0.88	0.22	62,62,62,62	0
54	MG	2A	3271	1/1	0.88	0.39	43,43,43,43	0
54	MG	1a	3133	1/1	0.88	0.12	67,67,67,67	0
54	MG	2A	3528	1/1	0.88	0.17	39,39,39,39	0
54	MG	2A	3275	1/1	0.88	0.24	39,39,39,39	0
54	MG	1h	201	1/1	0.89	0.20	29,29,29,29	0
54	MG	2A	3580	1/1	0.89	0.10	45,45,45,45	0
54	MG	2A	3187	1/1	0.89	0.18	55,55,55,55	0
54	MG	1A	3630	1/1	0.89	0.12	45,45,45,45	0
54	MG	1A	3436	1/1	0.89	0.17	18,18,18,18	0
54	MG	2A	3587	1/1	0.89	0.25	70,70,70,70	0
54	MG	2N	3801	1/1	0.89	0.08	54,54,54,54	0
54	MG	2A	3590	1/1	0.89	0.10	45,45,45,45	0
54	MG	1A	3572	1/1	0.89	0.19	43,43,43,43	0
54	MG	1A	3789	1/1	0.89	0.19	37,37,37,37	0
54	MG	2A	3597	1/1	0.89	0.07	66,66,66,66	0
54	MG	1a	3153	1/1	0.89	0.13	60,60,60,60	0
54	MG	1A	3146	1/1	0.89	0.12	39,39,39,39	0
54	MG	1A	3992	1/1	0.89	0.37	46,46,46,46	0
54	MG	2A	3204	1/1	0.89	0.26	41,41,41,41	0
54	MG	2I	102	1/1	0.89	0.14	63,63,63,63	0
54	MG	2A	3606	1/1	0.89	0.08	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3408	1/1	0.89	0.17	26,26,26,26	0
54	MG	2A	3611	1/1	0.89	0.11	32,32,32,32	0
54	MG	2A	3012	1/1	0.89	0.48	54,54,54,54	0
54	MG	2A	3613	1/1	0.89	0.14	25,25,25,25	0
54	MG	2A	3618	1/1	0.89	0.12	64,64,64,64	0
54	MG	1a	3171	1/1	0.89	0.10	72,72,72,72	0
54	MG	2A	3621	1/1	0.89	0.24	47,47,47,47	0
54	MG	2A	3210	1/1	0.89	0.13	33,33,33,33	0
54	MG	2A	3213	1/1	0.89	0.19	65,65,65,65	0
54	MG	1A	3898	1/1	0.89	0.22	33,33,33,33	0
54	MG	2A	3444	1/1	0.89	0.62	46,46,46,46	0
54	MG	2A	3630	1/1	0.89	0.15	49,49,49,49	0
54	MG	1A	3711	1/1	0.89	0.15	60,60,60,60	0
54	MG	1A	3300	1/1	0.89	0.26	46,46,46,46	0
54	MG	2A	3046	1/1	0.89	0.15	55,55,55,55	0
54	MG	1A	4001	1/1	0.89	0.29	67,67,67,67	0
54	MG	2a	3043	1/1	0.89	0.10	59,59,59,59	0
54	MG	1A	3652	1/1	0.89	0.73	40,40,40,40	0
54	MG	1A	3331	1/1	0.89	0.15	48,48,48,48	0
54	MG	1A	3729	1/1	0.89	0.10	33,33,33,33	0
54	MG	1a	3191	1/1	0.89	0.16	58,58,58,58	0
54	MG	2A	3063	1/1	0.89	0.29	46,46,46,46	0
54	MG	2a	3056	1/1	0.89	0.12	47,47,47,47	0
54	MG	1a	3194	1/1	0.89	0.08	56,56,56,56	0
54	MG	1A	3927	1/1	0.89	0.17	15,15,15,15	0
54	MG	2A	3243	1/1	0.89	0.21	43,43,43,43	0
54	MG	2A	3244	1/1	0.89	0.22	45,45,45,45	0
54	MG	2a	3068	1/1	0.89	0.12	72,72,72,72	0
54	MG	2A	3068	1/1	0.89	0.10	35,35,35,35	0
54	MG	2A	3069	1/1	0.89	0.31	55,55,55,55	0
54	MG	1A	3928	1/1	0.89	0.30	37,37,37,37	0
54	MG	1a	3061	1/1	0.89	0.30	59,59,59,59	0
54	MG	2a	3073	1/1	0.89	0.14	67,67,67,67	0
54	MG	2A	3260	1/1	0.89	0.17	50,50,50,50	0
54	MG	2a	3075	1/1	0.89	0.11	51,51,51,51	0
54	MG	2A	3677	1/1	0.89	0.17	53,53,53,53	0
54	MG	10	103	1/1	0.89	0.17	50,50,50,50	0
54	MG	2A	3679	1/1	0.89	0.14	30,30,30,30	0
54	MG	2A	3486	1/1	0.89	0.08	50,50,50,50	0
54	MG	2a	3090	1/1	0.89	0.12	63,63,63,63	0
54	MG	2A	3683	1/1	0.89	0.07	58,58,58,58	0
54	MG	1A	3135	1/1	0.89	0.25	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1a	3207	1/1	0.89	0.09	56,56,56,56	0
54	MG	1A	3603	1/1	0.89	0.09	28,28,28,28	0
54	MG	2A	3688	1/1	0.89	0.09	42,42,42,42	0
54	MG	2a	3102	1/1	0.89	0.08	56,56,56,56	0
54	MG	1A	3530	1/1	0.89	0.19	14,14,14,14	0
54	MG	2A	3096	1/1	0.89	0.29	77,77,77,77	0
54	MG	2a	3107	1/1	0.89	0.19	69,69,69,69	0
54	MG	1A	3276	1/1	0.89	0.12	51,51,51,51	0
54	MG	1a	3076	1/1	0.89	0.25	56,56,56,56	0
54	MG	2A	3703	1/1	0.89	0.10	55,55,55,55	0
54	MG	2A	3285	1/1	0.89	0.12	50,50,50,50	0
54	MG	2A	3711	1/1	0.89	0.09	58,58,58,58	0
54	MG	2A	3712	1/1	0.89	0.14	45,45,45,45	0
54	MG	2A	3714	1/1	0.89	0.20	39,39,39,39	0
54	MG	2A	3100	1/1	0.89	0.08	53,53,53,53	0
54	MG	2A	3112	1/1	0.89	0.27	50,50,50,50	0
54	MG	1a	3238	1/1	0.89	0.10	54,54,54,54	0
54	MG	1A	3940	1/1	0.89	0.29	50,50,50,50	0
54	MG	1A	3606	1/1	0.89	0.18	33,33,33,33	0
54	MG	2A	3311	1/1	0.89	0.14	49,49,49,49	0
54	MG	2a	3151	1/1	0.89	0.17	74,74,74,74	0
54	MG	2A	3313	1/1	0.89	0.15	53,53,53,53	0
54	MG	2a	3153	1/1	0.89	0.07	67,67,67,67	0
54	MG	2A	3535	1/1	0.89	0.14	43,43,43,43	0
54	MG	1a	3245	1/1	0.89	0.13	31,31,31,31	0
54	MG	1A	3949	1/1	0.89	0.10	31,31,31,31	0
54	MG	1A	3480	1/1	0.89	0.19	37,37,37,37	0
54	MG	2A	3750	1/1	0.89	0.07	45,45,45,45	0
54	MG	2A	3752	1/1	0.89	0.17	51,51,51,51	0
54	MG	2a	3171	1/1	0.89	0.07	68,68,68,68	0
54	MG	1A	3954	1/1	0.89	0.17	50,50,50,50	0
54	MG	1a	3093	1/1	0.89	0.15	43,43,43,43	0
54	MG	1B	208	1/1	0.89	0.17	45,45,45,45	0
54	MG	2B	202	1/1	0.89	0.23	70,70,70,70	0
54	MG	1B	209	1/1	0.89	0.32	55,55,55,55	0
54	MG	1A	3183	1/1	0.89	0.73	32,32,32,32	0
54	MG	1A	3430	1/1	0.89	0.15	26,26,26,26	0
54	MG	2A	3157	1/1	0.89	0.20	40,40,40,40	0
54	MG	2A	3559	1/1	0.89	0.06	57,57,57,57	0
54	MG	1A	3067	1/1	0.89	0.54	35,35,35,35	0
54	MG	1A	3756	1/1	0.89	0.11	47,47,47,47	0
54	MG	2B	218	1/1	0.89	0.09	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1a	3120	1/1	0.89	0.13	82,82,82,82	0
54	MG	1a	3017	1/1	0.89	0.15	60,60,60,60	0
54	MG	1a	3127	1/1	0.89	0.21	65,65,65,65	0
54	MG	1A	3628	1/1	0.89	0.26	35,35,35,35	0
54	MG	2D	312	1/1	0.89	0.20	46,46,46,46	0
54	MG	2A	3173	1/1	0.89	0.38	45,45,45,45	0
54	MG	1a	3056	1/1	0.90	0.13	38,38,38,38	0
54	MG	1A	3943	1/1	0.90	0.10	41,41,41,41	0
54	MG	1D	305	1/1	0.90	0.16	31,31,31,31	0
54	MG	1A	3127	1/1	0.90	0.11	42,42,42,42	0
54	MG	1A	3477	1/1	0.90	0.10	44,44,44,44	0
54	MG	2A	3347	1/1	0.90	0.11	31,31,31,31	0
54	MG	1A	3031	1/1	0.90	0.14	17,17,17,17	0
54	MG	1A	3804	1/1	0.90	0.53	55,55,55,55	0
54	MG	1a	3257	1/1	0.90	0.27	64,64,64,64	0
54	MG	1A	3963	1/1	0.90	0.17	56,56,56,56	0
54	MG	2R	201	1/1	0.90	0.45	47,47,47,47	0
54	MG	2A	3593	1/1	0.90	0.23	45,45,45,45	0
54	MG	1A	3806	1/1	0.90	0.18	41,41,41,41	0
54	MG	2A	3370	1/1	0.90	0.09	44,44,44,44	0
54	MG	1G	202	1/1	0.90	0.16	61,61,61,61	0
54	MG	2I	101	1/1	0.90	0.35	49,49,49,49	0
54	MG	2A	3169	1/1	0.90	0.15	68,68,68,68	0
54	MG	1G	203	1/1	0.90	0.07	52,52,52,52	0
54	MG	2A	3384	1/1	0.90	0.15	61,61,61,61	0
54	MG	1a	3272	1/1	0.90	0.07	60,60,60,60	0
54	MG	2A	3389	1/1	0.90	0.16	25,25,25,25	0
54	MG	2A	3390	1/1	0.90	0.14	23,23,23,23	0
54	MG	1A	3278	1/1	0.90	0.24	26,26,26,26	0
54	MG	2a	3009	1/1	0.90	0.13	67,67,67,67	0
54	MG	1a	3274	1/1	0.90	0.19	58,58,58,58	0
54	MG	2A	3185	1/1	0.90	0.10	57,57,57,57	0
54	MG	1A	3221	1/1	0.90	0.30	40,40,40,40	0
54	MG	2a	3023	1/1	0.90	0.25	51,51,51,51	0
54	MG	1A	3094	1/1	0.90	0.23	27,27,27,27	0
54	MG	2A	3188	1/1	0.90	0.12	56,56,56,56	0
54	MG	2A	3415	1/1	0.90	0.12	63,63,63,63	0
54	MG	1A	3345	1/1	0.90	0.17	21,21,21,21	0
54	MG	1A	3824	1/1	0.90	0.20	51,51,51,51	0
54	MG	2a	3035	1/1	0.90	0.10	50,50,50,50	0
54	MG	1A	3977	1/1	0.90	0.12	48,48,48,48	0
54	MG	2A	3430	1/1	0.90	0.21	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2a	3040	1/1	0.90	0.11	50,50,50,50	0
54	MG	2A	3431	1/1	0.90	0.28	74,74,74,74	0
54	MG	2A	3432	1/1	0.90	0.28	39,39,39,39	0
54	MG	1a	3107	1/1	0.90	0.16	63,63,63,63	0
54	MG	1g	203	1/1	0.90	0.54	57,57,57,57	0
54	MG	2A	3642	1/1	0.90	0.19	51,51,51,51	0
54	MG	1A	3497	1/1	0.90	0.20	24,24,24,24	0
54	MG	2A	3438	1/1	0.90	0.19	48,48,48,48	0
54	MG	2A	3647	1/1	0.90	0.14	65,65,65,65	0
54	MG	2a	3058	1/1	0.90	0.12	52,52,52,52	0
54	MG	2A	3650	1/1	0.90	0.16	52,52,52,52	0
54	MG	2A	3201	1/1	0.90	0.14	53,53,53,53	0
54	MG	1A	3287	1/1	0.90	0.13	62,62,62,62	0
54	MG	10	102	1/1	0.90	0.19	38,38,38,38	0
54	MG	1A	3850	1/1	0.90	0.11	34,34,34,34	0
54	MG	1A	3987	1/1	0.90	0.08	39,39,39,39	0
54	MG	1A	3851	1/1	0.90	0.19	24,24,24,24	0
54	MG	1y	204	1/1	0.90	0.16	63,63,63,63	0
54	MG	1a	3124	1/1	0.90	0.09	64,64,64,64	0
54	MG	1A	3056	1/1	0.90	0.14	55,55,55,55	0
54	MG	1A	3007	1/1	0.90	0.14	41,41,41,41	0
54	MG	2A	3218	1/1	0.90	0.16	63,63,63,63	0
54	MG	2A	3676	1/1	0.90	0.22	72,72,72,72	0
54	MG	1A	3618	1/1	0.90	0.11	28,28,28,28	0
54	MG	1A	3176	1/1	0.90	0.12	59,59,59,59	0
54	MG	2A	3024	1/1	0.90	0.18	51,51,51,51	0
54	MG	1a	3138	1/1	0.90	0.10	52,52,52,52	0
54	MG	2A	3035	1/1	0.90	0.15	38,38,38,38	0
54	MG	2a	3095	1/1	0.90	0.09	62,62,62,62	0
54	MG	1A	3247	1/1	0.90	0.25	35,35,35,35	0
54	MG	2A	3042	1/1	0.90	0.09	43,43,43,43	0
54	MG	2A	3236	1/1	0.90	0.36	35,35,35,35	0
54	MG	1A	3733	1/1	0.90	0.74	32,32,32,32	0
54	MG	1A	3517	1/1	0.90	0.12	35,35,35,35	0
54	MG	1A	3432	1/1	0.90	0.14	21,21,21,21	0
54	MG	1A	3880	1/1	0.90	0.14	47,47,47,47	0
54	MG	2A	3697	1/1	0.90	0.17	48,48,48,48	0
54	MG	2a	3109	1/1	0.90	0.11	63,63,63,63	0
54	MG	1A	3531	1/1	0.90	0.14	32,32,32,32	0
54	MG	2a	3113	1/1	0.90	0.15	53,53,53,53	0
54	MG	2A	3245	1/1	0.90	0.36	42,42,42,42	0
54	MG	1A	3638	1/1	0.90	0.15	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1a	3172	1/1	0.90	0.09	66,66,66,66	0
54	MG	1a	3175	1/1	0.90	0.14	54,54,54,54	0
54	MG	2A	3255	1/1	0.90	0.54	57,57,57,57	0
54	MG	1A	3369	1/1	0.90	0.14	19,19,19,19	0
54	MG	1A	3891	1/1	0.90	0.20	25,25,25,25	0
54	MG	1A	4027	1/1	0.90	0.25	42,42,42,42	0
54	MG	1A	3177	1/1	0.90	0.72	38,38,38,38	0
54	MG	2A	3517	1/1	0.90	0.14	69,69,69,69	0
54	MG	2A	3728	1/1	0.90	0.07	40,40,40,40	0
54	MG	2A	3071	1/1	0.90	0.16	34,34,34,34	0
54	MG	2A	3267	1/1	0.90	0.10	47,47,47,47	0
54	MG	2A	3525	1/1	0.90	0.31	62,62,62,62	0
54	MG	1A	3438	1/1	0.90	0.23	21,21,21,21	0
54	MG	1A	3545	1/1	0.90	0.30	50,50,50,50	0
54	MG	2a	3159	1/1	0.90	0.19	61,61,61,61	0
54	MG	1A	4034	1/1	0.90	0.08	50,50,50,50	0
54	MG	2A	3277	1/1	0.90	0.11	49,49,49,49	0
54	MG	1A	3755	1/1	0.90	0.15	30,30,30,30	0
54	MG	1A	3264	1/1	0.90	0.25	15,15,15,15	0
54	MG	2A	3538	1/1	0.90	0.35	67,67,67,67	0
54	MG	1a	3195	1/1	0.90	0.22	62,62,62,62	0
54	MG	2B	201	1/1	0.90	0.09	73,73,73,73	0
54	MG	2A	3543	1/1	0.90	0.37	63,63,63,63	0
54	MG	1A	3758	1/1	0.90	0.15	31,31,31,31	0
54	MG	1A	3452	1/1	0.90	0.14	42,42,42,42	0
54	MG	1A	3762	1/1	0.90	0.09	51,51,51,51	0
54	MG	2A	3550	1/1	0.90	0.14	25,25,25,25	0
54	MG	2A	3298	1/1	0.90	0.13	48,48,48,48	0
54	MG	1A	3322	1/1	0.90	0.21	51,51,51,51	0
54	MG	1A	3679	1/1	0.90	0.11	41,41,41,41	0
54	MG	2B	215	1/1	0.90	0.31	74,74,74,74	0
54	MG	1A	3782	1/1	0.90	0.07	19,19,19,19	0
54	MG	2A	3114	1/1	0.90	0.06	60,60,60,60	0
54	MG	2n	101	1/1	0.90	0.11	65,65,65,65	0
56	MPD	1T	207	8/8	0.90	0.29	69,71,74,77	0
54	MG	1A	3214	1/1	0.90	0.11	37,37,37,37	0
54	MG	1a	3217	1/1	0.90	0.19	72,72,72,72	0
54	MG	1A	3573	1/1	0.90	0.11	34,34,34,34	0
54	MG	1A	3326	1/1	0.90	0.17	48,48,48,48	0
54	MG	2A	3572	1/1	0.90	0.14	62,62,62,62	0
54	MG	1A	3215	1/1	0.90	0.44	23,23,23,23	0
54	MG	2A	3748	1/1	0.91	0.09	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1a	3074	1/1	0.91	0.12	55,55,55,55	0
54	MG	1d	303	1/1	0.91	0.14	45,45,45,45	0
54	MG	2A	3483	1/1	0.91	0.08	48,48,48,48	0
54	MG	2A	3217	1/1	0.91	0.23	34,34,34,34	0
54	MG	1A	3193	1/1	0.91	0.13	68,68,68,68	0
54	MG	2A	3219	1/1	0.91	0.19	50,50,50,50	0
54	MG	1D	308	1/1	0.91	0.20	45,45,45,45	0
54	MG	2B	203	1/1	0.91	0.12	61,61,61,61	0
54	MG	1e	202	1/1	0.91	0.46	55,55,55,55	0
54	MG	1a	3078	1/1	0.91	0.14	62,62,62,62	0
54	MG	1D	309	1/1	0.91	0.44	25,25,25,25	0
54	MG	1A	3773	1/1	0.91	0.18	64,64,64,64	0
54	MG	1A	3504	1/1	0.91	0.09	51,51,51,51	0
54	MG	2A	3503	1/1	0.91	0.41	76,76,76,76	0
54	MG	2A	3505	1/1	0.91	0.10	41,41,41,41	0
54	MG	1a	3088	1/1	0.91	0.45	58,58,58,58	0
54	MG	2B	217	1/1	0.91	0.18	71,71,71,71	0
54	MG	1A	3650	1/1	0.91	0.15	27,27,27,27	0
54	MG	1F	303	1/1	0.91	0.55	30,30,30,30	0
54	MG	2A	3516	1/1	0.91	0.18	46,46,46,46	0
54	MG	1A	3651	1/1	0.91	0.21	32,32,32,32	0
54	MG	1A	3945	1/1	0.91	0.12	41,41,41,41	0
54	MG	1A	3508	1/1	0.91	0.06	59,59,59,59	0
54	MG	2A	3002	1/1	0.91	0.13	44,44,44,44	0
54	MG	1A	3791	1/1	0.91	0.21	20,20,20,20	0
54	MG	1A	3417	1/1	0.91	0.27	20,20,20,20	0
54	MG	1A	3267	1/1	0.91	0.69	34,34,34,34	0
54	MG	2A	3250	1/1	0.91	0.14	49,49,49,49	0
54	MG	1A	3796	1/1	0.91	0.59	39,39,39,39	0
54	MG	2A	3020	1/1	0.91	0.51	31,31,31,31	0
54	MG	1A	3155	1/1	0.91	0.19	40,40,40,40	0
54	MG	2A	3258	1/1	0.91	0.62	59,59,59,59	0
54	MG	2A	3025	1/1	0.91	0.43	58,58,58,58	0
54	MG	1A	3429	1/1	0.91	0.16	58,58,58,58	0
54	MG	2A	3546	1/1	0.91	0.11	53,53,53,53	0
54	MG	2A	3263	1/1	0.91	0.13	44,44,44,44	0
54	MG	2A	3030	1/1	0.91	0.49	44,44,44,44	0
54	MG	1A	3033	1/1	0.91	0.29	35,35,35,35	0
54	MG	1A	3971	1/1	0.91	0.16	37,37,37,37	0
54	MG	1A	3209	1/1	0.91	0.28	34,34,34,34	0
54	MG	1U	207	1/1	0.91	0.25	42,42,42,42	0
54	MG	1A	3162	1/1	0.91	0.42	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	27	102	1/1	0.91	0.84	36,36,36,36	0
54	MG	1A	3434	1/1	0.91	0.17	12,12,12,12	0
54	MG	2A	3051	1/1	0.91	0.09	53,53,53,53	0
54	MG	2a	3003	1/1	0.91	0.17	51,51,51,51	0
54	MG	2A	3280	1/1	0.91	0.45	57,57,57,57	0
54	MG	2A	3052	1/1	0.91	0.11	53,53,53,53	0
54	MG	1A	3808	1/1	0.91	0.16	60,60,60,60	0
54	MG	1A	3555	1/1	0.91	0.12	58,58,58,58	0
54	MG	1a	3144	1/1	0.91	0.07	52,52,52,52	0
54	MG	11	104	1/1	0.91	0.11	33,33,33,33	0
54	MG	2A	3293	1/1	0.91	0.14	39,39,39,39	0
54	MG	2a	3019	1/1	0.91	0.25	51,51,51,51	0
54	MG	2A	3295	1/1	0.91	0.10	57,57,57,57	0
54	MG	13	102	1/1	0.91	0.19	18,18,18,18	0
54	MG	2A	3299	1/1	0.91	0.11	53,53,53,53	0
54	MG	2A	3301	1/1	0.91	0.17	27,27,27,27	0
54	MG	1a	3156	1/1	0.91	0.28	60,60,60,60	0
54	MG	2a	3029	1/1	0.91	0.31	63,63,63,63	0
54	MG	13	103	1/1	0.91	0.17	37,37,37,37	0
54	MG	2A	3310	1/1	0.91	0.10	37,37,37,37	0
54	MG	13	105	1/1	0.91	0.23	41,41,41,41	0
54	MG	1A	3556	1/1	0.91	0.34	27,27,27,27	0
54	MG	2a	3038	1/1	0.91	0.24	70,70,70,70	0
54	MG	15	105	1/1	0.91	0.32	18,18,18,18	0
54	MG	1A	3060	1/1	0.91	0.22	27,27,27,27	0
54	MG	1A	3985	1/1	0.91	0.12	28,28,28,28	0
54	MG	2a	3042	1/1	0.91	0.07	49,49,49,49	0
54	MG	2A	3326	1/1	0.91	0.11	51,51,51,51	0
54	MG	1A	3821	1/1	0.91	0.17	48,48,48,48	0
54	MG	2A	3334	1/1	0.91	0.13	34,34,34,34	0
54	MG	1A	3062	1/1	0.91	0.35	33,33,33,33	0
54	MG	1a	3180	1/1	0.91	0.06	63,63,63,63	0
54	MG	2A	3090	1/1	0.91	0.22	33,33,33,33	0
54	MG	1A	3439	1/1	0.91	0.11	19,19,19,19	0
54	MG	1A	3695	1/1	0.91	0.17	36,36,36,36	0
54	MG	1A	3849	1/1	0.91	0.12	43,43,43,43	0
54	MG	1A	3442	1/1	0.91	0.22	21,21,21,21	0
54	MG	2a	3064	1/1	0.91	0.11	73,73,73,73	0
54	MG	2A	3348	1/1	0.91	0.12	24,24,24,24	0
54	MG	1A	3218	1/1	0.91	0.64	20,20,20,20	0
54	MG	1A	3576	1/1	0.91	0.10	53,53,53,53	0
54	MG	2A	3104	1/1	0.91	0.17	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3361	1/1	0.91	0.08	35,35,35,35	0
54	MG	1A	3587	1/1	0.91	0.10	63,63,63,63	0
54	MG	1A	3098	1/1	0.91	0.12	26,26,26,26	0
54	MG	1a	3198	1/1	0.91	0.17	73,73,73,73	0
54	MG	1A	3373	1/1	0.91	0.17	24,24,24,24	0
54	MG	1A	3719	1/1	0.91	0.35	34,34,34,34	0
54	MG	1A	3375	1/1	0.91	0.17	42,42,42,42	0
54	MG	1A	3464	1/1	0.91	0.15	45,45,45,45	0
54	MG	2A	3132	1/1	0.91	0.18	47,47,47,47	0
54	MG	1A	3145	1/1	0.91	0.56	28,28,28,28	0
54	MG	1A	3178	1/1	0.91	0.19	25,25,25,25	0
54	MG	1a	3210	1/1	0.91	0.15	58,58,58,58	0
54	MG	1a	3211	1/1	0.91	0.08	63,63,63,63	0
54	MG	1A	3881	1/1	0.91	0.13	30,30,30,30	0
54	MG	1a	3215	1/1	0.91	0.08	73,73,73,73	0
54	MG	2A	3657	1/1	0.91	0.06	65,65,65,65	0
54	MG	2A	3151	1/1	0.91	0.10	50,50,50,50	0
54	MG	2a	3101	1/1	0.91	0.13	63,63,63,63	0
54	MG	2A	3401	1/1	0.91	0.09	74,74,74,74	0
54	MG	2A	3402	1/1	0.91	0.15	62,62,62,62	0
54	MG	2A	3405	1/1	0.91	0.13	54,54,54,54	0
54	MG	2a	3105	1/1	0.91	0.11	80,80,80,80	0
54	MG	1A	3224	1/1	0.91	0.45	32,32,32,32	0
54	MG	2A	3667	1/1	0.91	0.10	58,58,58,58	0
54	MG	2A	3668	1/1	0.91	0.14	49,49,49,49	0
54	MG	2A	3413	1/1	0.91	0.09	56,56,56,56	0
54	MG	1A	3180	1/1	0.91	0.85	34,34,34,34	0
54	MG	2A	3159	1/1	0.91	0.49	55,55,55,55	0
54	MG	1a	3220	1/1	0.91	0.10	63,63,63,63	0
54	MG	1A	3050	1/1	0.91	0.45	30,30,30,30	0
54	MG	2A	3429	1/1	0.91	0.42	44,44,44,44	0
54	MG	2a	3125	1/1	0.91	0.10	66,66,66,66	0
54	MG	2a	3128	1/1	0.91	0.05	61,61,61,61	0
54	MG	1a	3232	1/1	0.91	0.14	31,31,31,31	0
54	MG	1A	3609	1/1	0.91	0.11	26,26,26,26	0
54	MG	2A	3682	1/1	0.91	0.10	21,21,21,21	0
54	MG	2a	3135	1/1	0.91	0.14	62,62,62,62	0
54	MG	1a	3035	1/1	0.91	0.17	57,57,57,57	0
54	MG	1A	3147	1/1	0.91	0.18	28,28,28,28	0
54	MG	1A	4045	1/1	0.91	0.26	46,46,46,46	0
54	MG	2a	3148	1/1	0.91	0.12	63,63,63,63	0
54	MG	1a	3244	1/1	0.91	0.13	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2a	3150	1/1	0.91	0.08	64,64,64,64	0
54	MG	1a	3041	1/1	0.91	0.14	68,68,68,68	0
54	MG	2A	3689	1/1	0.91	0.07	45,45,45,45	0
54	MG	1A	3896	1/1	0.91	0.12	45,45,45,45	0
54	MG	1a	3044	1/1	0.91	0.10	57,57,57,57	0
54	MG	2A	3692	1/1	0.91	0.07	70,70,70,70	0
54	MG	1A	3748	1/1	0.91	0.38	61,61,61,61	0
54	MG	1A	3489	1/1	0.91	0.13	44,44,44,44	0
54	MG	1a	3258	1/1	0.91	0.26	55,55,55,55	0
54	MG	2a	3166	1/1	0.91	0.13	55,55,55,55	0
54	MG	1a	3259	1/1	0.91	0.10	48,48,48,48	0
54	MG	1A	3051	1/1	0.91	0.56	36,36,36,36	0
54	MG	2A	3710	1/1	0.91	0.10	50,50,50,50	0
54	MG	1a	3267	1/1	0.91	0.19	54,54,54,54	0
54	MG	2a	3175	1/1	0.91	0.07	68,68,68,68	0
54	MG	1A	3396	1/1	0.91	0.12	37,37,37,37	0
54	MG	1A	3026	1/1	0.91	0.64	27,27,27,27	0
54	MG	1A	3249	1/1	0.91	0.35	27,27,27,27	0
54	MG	1B	218	1/1	0.91	0.13	31,31,31,31	0
54	MG	2A	3459	1/1	0.91	0.17	53,53,53,53	0
54	MG	1A	3255	1/1	0.91	0.10	39,39,39,39	0
54	MG	1A	3333	1/1	0.91	0.10	45,45,45,45	0
54	MG	1A	3038	1/1	0.91	0.17	28,28,28,28	0
54	MG	2A	3730	1/1	0.91	1.34	57,57,57,57	0
54	MG	2A	3731	1/1	0.91	0.07	70,70,70,70	0
54	MG	2A	3464	1/1	0.91	0.39	44,44,44,44	0
54	MG	2A	3467	1/1	0.91	0.08	38,38,38,38	0
54	MG	1a	3279	1/1	0.91	0.11	68,68,68,68	0
54	MG	2A	3735	1/1	0.91	0.13	46,46,46,46	0
54	MG	2A	3211	1/1	0.91	0.25	41,41,41,41	0
54	MG	2A	3737	1/1	0.91	0.11	67,67,67,67	0
54	MG	2A	3740	1/1	0.91	0.51	48,48,48,48	0
54	MG	2A	3212	1/1	0.91	0.20	45,45,45,45	0
58	ZN	2Y	202	1/1	0.91	0.06	101,101,101,101	0
54	MG	1A	3336	1/1	0.91	0.18	47,47,47,47	0
54	MG	2A	3511	1/1	0.92	0.11	66,66,66,66	0
54	MG	2A	3021	1/1	0.92	0.60	42,42,42,42	0
54	MG	2A	3513	1/1	0.92	0.10	40,40,40,40	0
54	MG	2B	209	1/1	0.92	0.24	57,57,57,57	0
54	MG	2A	3514	1/1	0.92	0.16	64,64,64,64	0
54	MG	1W	201	1/1	0.92	0.28	34,34,34,34	0
54	MG	1A	3633	1/1	0.92	0.17	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3841	1/1	0.92	0.77	43,43,43,43	0
54	MG	2A	3028	1/1	0.92	0.24	41,41,41,41	0
54	MG	1a	3132	1/1	0.92	0.10	53,53,53,53	0
54	MG	1A	3843	1/1	0.92	0.10	31,31,31,31	0
54	MG	2D	301	1/1	0.92	0.59	40,40,40,40	0
54	MG	2A	3527	1/1	0.92	0.15	22,22,22,22	0
54	MG	10	105	1/1	0.92	0.21	54,54,54,54	0
54	MG	2A	3040	1/1	0.92	0.11	48,48,48,48	0
54	MG	1A	3730	1/1	0.92	0.67	30,30,30,30	0
54	MG	2A	3043	1/1	0.92	0.09	42,42,42,42	0
54	MG	1a	3141	1/1	0.92	0.16	64,64,64,64	0
54	MG	2E	303	1/1	0.92	0.28	51,51,51,51	0
54	MG	1A	3845	1/1	0.92	0.11	42,42,42,42	0
54	MG	1A	3096	1/1	0.92	0.18	42,42,42,42	0
54	MG	2F	303	1/1	0.92	0.69	49,49,49,49	0
54	MG	1a	3145	1/1	0.92	0.19	57,57,57,57	0
54	MG	1a	3149	1/1	0.92	0.16	64,64,64,64	0
54	MG	1A	3246	1/1	0.92	0.25	26,26,26,26	0
54	MG	1A	3990	1/1	0.92	0.28	35,35,35,35	0
54	MG	1a	3154	1/1	0.92	0.15	40,40,40,40	0
54	MG	14	101	1/1	0.92	0.08	71,71,71,71	0
54	MG	1a	3161	1/1	0.92	0.13	70,70,70,70	0
54	MG	1A	3071	1/1	0.92	0.24	34,34,34,34	0
54	MG	1A	3641	1/1	0.92	0.23	15,15,15,15	0
54	MG	1A	3361	1/1	0.92	0.07	45,45,45,45	0
54	MG	1A	3571	1/1	0.92	0.11	44,44,44,44	0
54	MG	1A	3745	1/1	0.92	0.12	48,48,48,48	0
54	MG	1A	3864	1/1	0.92	0.35	38,38,38,38	0
54	MG	2A	3563	1/1	0.92	0.87	61,61,61,61	0
54	MG	20	102	1/1	0.92	0.11	54,54,54,54	0
54	MG	1A	3867	1/1	0.92	0.16	38,38,38,38	0
54	MG	2A	3307	1/1	0.92	0.09	28,28,28,28	0
54	MG	1A	3747	1/1	0.92	0.18	32,32,32,32	0
54	MG	2A	3567	1/1	0.92	0.21	41,41,41,41	0
54	MG	2A	3570	1/1	0.92	0.13	51,51,51,51	0
54	MG	1A	4005	1/1	0.92	0.08	61,61,61,61	0
54	MG	1A	4007	1/1	0.92	0.13	73,73,73,73	0
54	MG	1A	3317	1/1	0.92	0.18	47,47,47,47	0
54	MG	1A	3137	1/1	0.92	0.50	36,36,36,36	0
54	MG	1A	4016	1/1	0.92	0.18	25,25,25,25	0
54	MG	2a	3008	1/1	0.92	0.21	36,36,36,36	0
54	MG	1a	3008	1/1	0.92	0.13	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2a	3010	1/1	0.92	0.12	66,66,66,66	0
54	MG	1A	3014	1/1	0.92	0.12	46,46,46,46	0
54	MG	1A	3657	1/1	0.92	0.12	68,68,68,68	0
54	MG	2a	3016	1/1	0.92	0.18	65,65,65,65	0
54	MG	1a	3014	1/1	0.92	0.07	55,55,55,55	0
54	MG	2A	3586	1/1	0.92	0.10	41,41,41,41	0
54	MG	2A	3101	1/1	0.92	0.53	48,48,48,48	0
54	MG	2A	3336	1/1	0.92	0.15	26,26,26,26	0
54	MG	1a	3015	1/1	0.92	0.20	63,63,63,63	0
54	MG	1A	3065	1/1	0.92	0.20	44,44,44,44	0
54	MG	1A	3580	1/1	0.92	0.15	46,46,46,46	0
54	MG	2a	3031	1/1	0.92	0.14	56,56,56,56	0
54	MG	1A	4029	1/1	0.92	0.19	43,43,43,43	0
54	MG	2A	3118	1/1	0.92	0.08	39,39,39,39	0
54	MG	1A	3078	1/1	0.92	0.17	27,27,27,27	0
54	MG	1a	3025	1/1	0.92	0.13	44,44,44,44	0
54	MG	2A	3603	1/1	0.92	0.10	32,32,32,32	0
54	MG	2A	3349	1/1	0.92	0.30	57,57,57,57	0
54	MG	1A	3105	1/1	0.92	0.44	37,37,37,37	0
54	MG	2A	3354	1/1	0.92	0.11	40,40,40,40	0
54	MG	1A	3216	1/1	0.92	0.12	43,43,43,43	0
54	MG	1A	3059	1/1	0.92	0.22	44,44,44,44	0
54	MG	1A	3149	1/1	0.92	0.39	36,36,36,36	0
54	MG	2a	3048	1/1	0.92	0.40	70,70,70,70	0
54	MG	2A	3617	1/1	0.92	0.09	57,57,57,57	0
54	MG	1A	3770	1/1	0.92	0.10	44,44,44,44	0
54	MG	1A	3771	1/1	0.92	0.13	32,32,32,32	0
54	MG	2A	3140	1/1	0.92	0.16	45,45,45,45	0
54	MG	1A	3772	1/1	0.92	0.11	42,42,42,42	0
54	MG	2A	3146	1/1	0.92	0.63	52,52,52,52	0
54	MG	2A	3147	1/1	0.92	0.17	27,27,27,27	0
54	MG	1A	3182	1/1	0.92	0.42	53,53,53,53	0
54	MG	2a	3063	1/1	0.92	0.23	77,77,77,77	0
54	MG	1A	3774	1/1	0.92	0.15	33,33,33,33	0
54	MG	1a	3225	1/1	0.92	0.09	67,67,67,67	0
54	MG	1a	3226	1/1	0.92	0.07	55,55,55,55	0
54	MG	1A	3917	1/1	0.92	0.15	58,58,58,58	0
54	MG	2A	3392	1/1	0.92	0.21	67,67,67,67	0
54	MG	1A	3777	1/1	0.92	0.16	41,41,41,41	0
54	MG	2A	3638	1/1	0.92	0.06	43,43,43,43	0
54	MG	2A	3639	1/1	0.92	0.11	40,40,40,40	0
54	MG	1A	3506	1/1	0.92	0.15	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3165	1/1	0.92	0.57	54,54,54,54	0
54	MG	1B	216	1/1	0.92	0.16	35,35,35,35	0
54	MG	1a	3049	1/1	0.92	0.13	38,38,38,38	0
54	MG	1A	3925	1/1	0.92	0.12	35,35,35,35	0
54	MG	1A	3447	1/1	0.92	0.09	48,48,48,48	0
54	MG	2A	3406	1/1	0.92	0.15	49,49,49,49	0
54	MG	1B	220	1/1	0.92	0.21	40,40,40,40	0
54	MG	1B	221	1/1	0.92	0.11	38,38,38,38	0
54	MG	2a	3094	1/1	0.92	0.13	38,38,38,38	0
54	MG	1a	3252	1/1	0.92	0.08	56,56,56,56	0
54	MG	2A	3420	1/1	0.92	0.24	59,59,59,59	0
54	MG	2A	3421	1/1	0.92	0.18	48,48,48,48	0
54	MG	2A	3422	1/1	0.92	0.14	42,42,42,42	0
54	MG	2A	3174	1/1	0.92	0.09	45,45,45,45	0
54	MG	2A	3179	1/1	0.92	0.12	52,52,52,52	0
54	MG	2A	3183	1/1	0.92	0.48	51,51,51,51	0
54	MG	1A	3515	1/1	0.92	0.14	53,53,53,53	0
54	MG	1A	3087	1/1	0.92	0.26	34,34,34,34	0
54	MG	1A	3932	1/1	0.92	0.10	34,34,34,34	0
54	MG	1A	3693	1/1	0.92	0.21	51,51,51,51	0
54	MG	1a	3262	1/1	0.92	0.11	52,52,52,52	0
54	MG	1a	3067	1/1	0.92	0.40	67,67,67,67	0
54	MG	2a	3111	1/1	0.92	0.25	55,55,55,55	0
54	MG	1D	303	1/1	0.92	0.34	46,46,46,46	0
54	MG	2A	3437	1/1	0.92	0.11	45,45,45,45	0
54	MG	2A	3681	1/1	0.92	0.12	36,36,36,36	0
54	MG	1a	3070	1/1	0.92	0.21	60,60,60,60	0
54	MG	2A	3198	1/1	0.92	0.13	38,38,38,38	0
54	MG	1A	3120	1/1	0.92	0.41	31,31,31,31	0
54	MG	2a	3124	1/1	0.92	0.13	56,56,56,56	0
54	MG	1A	3611	1/1	0.92	0.13	53,53,53,53	0
54	MG	2a	3126	1/1	0.92	0.20	48,48,48,48	0
54	MG	1A	3187	1/1	0.92	0.21	25,25,25,25	0
54	MG	1A	3069	1/1	0.92	0.76	25,25,25,25	0
54	MG	1A	3190	1/1	0.92	0.15	56,56,56,56	0
54	MG	1A	3802	1/1	0.92	0.11	39,39,39,39	0
54	MG	2A	3450	1/1	0.92	0.17	48,48,48,48	0
54	MG	1A	3947	1/1	0.92	0.11	39,39,39,39	0
54	MG	2a	3140	1/1	0.92	0.14	53,53,53,53	0
54	MG	2a	3142	1/1	0.92	0.08	62,62,62,62	0
54	MG	1b	301	1/1	0.92	0.19	64,64,64,64	0
54	MG	1a	3085	1/1	0.92	0.26	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3346	1/1	0.92	0.18	12,12,12,12	0
54	MG	1F	314	1/1	0.92	0.11	47,47,47,47	0
54	MG	1A	3708	1/1	0.92	0.17	28,28,28,28	0
54	MG	1a	3091	1/1	0.92	0.11	56,56,56,56	0
54	MG	1A	3623	1/1	0.92	0.45	33,33,33,33	0
54	MG	1A	3962	1/1	0.92	0.21	32,32,32,32	0
54	MG	1a	3094	1/1	0.92	0.10	56,56,56,56	0
54	MG	1a	3098	1/1	0.92	0.16	43,43,43,43	0
54	MG	1k	201	1/1	0.92	0.17	36,36,36,36	0
54	MG	2A	3471	1/1	0.92	0.11	68,68,68,68	0
54	MG	1A	3624	1/1	0.92	0.07	74,74,74,74	0
54	MG	1a	3103	1/1	0.92	0.14	57,57,57,57	0
54	MG	2A	3476	1/1	0.92	0.20	50,50,50,50	0
54	MG	2A	3225	1/1	0.92	0.25	45,45,45,45	0
54	MG	1A	3716	1/1	0.92	0.43	42,42,42,42	0
54	MG	2A	3480	1/1	0.92	0.21	63,63,63,63	0
54	MG	2A	3228	1/1	0.92	0.27	52,52,52,52	0
54	MG	2A	3482	1/1	0.92	0.21	38,38,38,38	0
54	MG	1o	101	1/1	0.92	0.20	49,49,49,49	0
54	MG	2a	3182	1/1	0.92	0.07	74,74,74,74	0
54	MG	1A	3295	1/1	0.92	0.11	46,46,46,46	0
54	MG	1a	3109	1/1	0.92	0.07	41,41,41,41	0
54	MG	2a	3185	1/1	0.92	0.09	45,45,45,45	0
54	MG	2A	3739	1/1	0.92	0.17	40,40,40,40	0
54	MG	1y	203	1/1	0.92	0.15	59,59,59,59	0
54	MG	1A	3969	1/1	0.92	0.09	51,51,51,51	0
54	MG	1A	3721	1/1	0.92	0.52	41,41,41,41	0
54	MG	2a	3196	1/1	0.92	0.19	68,68,68,68	0
54	MG	2A	3745	1/1	0.92	0.10	50,50,50,50	0
54	MG	2A	3746	1/1	0.92	0.08	71,71,71,71	0
54	MG	2f	201	1/1	0.92	0.10	53,53,53,53	0
54	MG	1a	3117	1/1	0.92	0.28	68,68,68,68	0
54	MG	1A	3816	1/1	0.92	0.22	47,47,47,47	0
54	MG	2A	3497	1/1	0.92	0.09	65,65,65,65	0
54	MG	1A	3549	1/1	0.92	0.14	57,57,57,57	0
54	MG	1A	3726	1/1	0.92	0.18	45,45,45,45	0
54	MG	1A	3413	1/1	0.92	0.12	24,24,24,24	0
57	ARG	1B	228	12/12	0.92	0.28	22,42,59,67	0
54	MG	2A	3757	1/1	0.92	0.10	46,46,46,46	0
54	MG	1a	3123	1/1	0.92	0.12	32,32,32,32	0
54	MG	2A	3249	1/1	0.92	0.73	46,46,46,46	0
54	MG	2A	3510	1/1	0.92	0.09	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	ZN	2n	102	1/1	0.92	0.08	93,93,93,93	0
54	MG	1A	3360	1/1	0.93	0.10	34,34,34,34	0
54	MG	1A	4039	1/1	0.93	0.30	34,34,34,34	0
54	MG	2A	3487	1/1	0.93	0.07	52,52,52,52	0
54	MG	1a	3261	1/1	0.93	0.06	55,55,55,55	0
54	MG	1a	3043	1/1	0.93	0.23	47,47,47,47	0
54	MG	1A	3648	1/1	0.93	0.08	33,33,33,33	0
54	MG	1A	4044	1/1	0.93	0.12	35,35,35,35	0
54	MG	1A	3541	1/1	0.93	0.13	52,52,52,52	0
54	MG	2B	208	1/1	0.93	0.09	57,57,57,57	0
54	MG	1A	4048	1/1	0.93	0.54	58,58,58,58	0
54	MG	1A	3892	1/1	0.93	0.14	55,55,55,55	0
54	MG	1A	3303	1/1	0.93	0.44	26,26,26,26	0
54	MG	1B	205	1/1	0.93	0.11	40,40,40,40	0
54	MG	1B	207	1/1	0.93	0.07	51,51,51,51	0
54	MG	2A	3507	1/1	0.93	0.38	53,53,53,53	0
54	MG	2A	3508	1/1	0.93	0.09	61,61,61,61	0
54	MG	1a	3058	1/1	0.93	0.09	57,57,57,57	0
54	MG	1a	3060	1/1	0.93	0.20	57,57,57,57	0
54	MG	1A	3240	1/1	0.93	0.18	56,56,56,56	0
54	MG	1A	3655	1/1	0.93	0.17	28,28,28,28	0
54	MG	1A	3368	1/1	0.93	0.14	51,51,51,51	0
54	MG	1a	3066	1/1	0.93	0.52	66,66,66,66	0
54	MG	1A	3899	1/1	0.93	0.08	59,59,59,59	0
54	MG	1A	3443	1/1	0.93	0.16	18,18,18,18	0
54	MG	2A	3237	1/1	0.93	0.32	43,43,43,43	0
54	MG	2A	3518	1/1	0.93	0.26	67,67,67,67	0
54	MG	1A	3903	1/1	0.93	0.38	41,41,41,41	0
54	MG	1f	201	1/1	0.93	0.22	61,61,61,61	0
54	MG	1A	3662	1/1	0.93	0.24	27,27,27,27	0
54	MG	2A	3526	1/1	0.93	0.32	45,45,45,45	0
54	MG	1A	3667	1/1	0.93	0.15	47,47,47,47	0
54	MG	1A	3445	1/1	0.93	0.09	20,20,20,20	0
54	MG	1A	3306	1/1	0.93	0.14	65,65,65,65	0
54	MG	1A	3566	1/1	0.93	0.16	27,27,27,27	0
54	MG	2A	3532	1/1	0.93	0.15	56,56,56,56	0
54	MG	1a	3081	1/1	0.93	0.17	53,53,53,53	0
54	MG	1A	3372	1/1	0.93	0.17	13,13,13,13	0
54	MG	1A	3787	1/1	0.93	0.13	32,32,32,32	0
54	MG	2R	202	1/1	0.93	0.30	30,30,30,30	0
54	MG	1t	201	1/1	0.93	0.15	67,67,67,67	0
54	MG	1A	3073	1/1	0.93	0.13	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3311	1/1	0.93	0.13	30,30,30,30	0
54	MG	1D	306	1/1	0.93	0.36	39,39,39,39	0
54	MG	1A	3790	1/1	0.93	0.13	28,28,28,28	0
54	MG	2A	3547	1/1	0.93	0.15	56,56,56,56	0
54	MG	1A	3934	1/1	0.93	0.12	33,33,33,33	0
54	MG	23	101	1/1	0.93	0.90	57,57,57,57	0
54	MG	1A	3684	1/1	0.93	0.08	48,48,48,48	0
54	MG	1A	3203	1/1	0.93	0.13	35,35,35,35	0
54	MG	1D	317	1/1	0.93	0.11	43,43,43,43	0
54	MG	1a	3095	1/1	0.93	0.10	60,60,60,60	0
54	MG	2A	3556	1/1	0.93	0.10	62,62,62,62	0
54	MG	1a	3097	1/1	0.93	0.16	55,55,55,55	0
54	MG	1A	3104	1/1	0.93	0.45	27,27,27,27	0
54	MG	1F	302	1/1	0.93	0.15	22,22,22,22	0
54	MG	1A	3320	1/1	0.93	0.14	52,52,52,52	0
54	MG	1A	3690	1/1	0.93	0.12	50,50,50,50	0
54	MG	1A	3092	1/1	0.93	0.37	32,32,32,32	0
54	MG	1A	3581	1/1	0.93	0.09	42,42,42,42	0
54	MG	1A	3583	1/1	0.93	0.15	36,36,36,36	0
54	MG	2A	3033	1/1	0.93	0.19	58,58,58,58	0
54	MG	2a	3017	1/1	0.93	0.12	51,51,51,51	0
54	MG	2A	3569	1/1	0.93	0.21	26,26,26,26	0
54	MG	1A	3584	1/1	0.93	0.12	42,42,42,42	0
54	MG	1A	3951	1/1	0.93	0.05	48,48,48,48	0
54	MG	2A	3291	1/1	0.93	0.09	51,51,51,51	0
54	MG	2A	3037	1/1	0.93	0.16	50,50,50,50	0
54	MG	2a	3026	1/1	0.93	0.12	43,43,43,43	0
54	MG	2A	3575	1/1	0.93	0.05	45,45,45,45	0
54	MG	2A	3576	1/1	0.93	0.11	56,56,56,56	0
54	MG	1A	3805	1/1	0.93	0.16	26,26,26,26	0
54	MG	1A	3586	1/1	0.93	0.17	12,12,12,12	0
54	MG	1A	3958	1/1	0.93	0.08	29,29,29,29	0
54	MG	1a	3121	1/1	0.93	0.12	62,62,62,62	0
54	MG	1P	204	1/1	0.93	0.29	47,47,47,47	0
54	MG	2A	3049	1/1	0.93	0.13	54,54,54,54	0
54	MG	1A	3251	1/1	0.93	0.31	34,34,34,34	0
54	MG	1Q	201	1/1	0.93	0.16	26,26,26,26	0
54	MG	1R	202	1/1	0.93	0.37	29,29,29,29	0
54	MG	1A	3093	1/1	0.93	0.23	29,29,29,29	0
54	MG	2A	3318	1/1	0.93	0.19	64,64,64,64	0
54	MG	1A	3809	1/1	0.93	0.18	41,41,41,41	0
54	MG	1R	206	1/1	0.93	0.20	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3812	1/1	0.93	0.11	59,59,59,59	0
54	MG	1T	206	1/1	0.93	0.25	48,48,48,48	0
54	MG	2A	3600	1/1	0.93	0.11	51,51,51,51	0
54	MG	2a	3053	1/1	0.93	0.11	54,54,54,54	0
54	MG	2A	3601	1/1	0.93	0.10	38,38,38,38	0
54	MG	2A	3327	1/1	0.93	0.14	40,40,40,40	0
54	MG	2a	3057	1/1	0.93	0.12	59,59,59,59	0
54	MG	1U	203	1/1	0.93	0.34	28,28,28,28	0
54	MG	2a	3060	1/1	0.93	0.14	46,46,46,46	0
54	MG	1A	3391	1/1	0.93	0.14	31,31,31,31	0
54	MG	2A	3067	1/1	0.93	0.24	37,37,37,37	0
54	MG	1A	3052	1/1	0.93	0.20	11,11,11,11	0
54	MG	1A	3815	1/1	0.93	0.18	26,26,26,26	0
54	MG	2A	3070	1/1	0.93	0.55	45,45,45,45	0
54	MG	1A	3328	1/1	0.93	0.09	54,54,54,54	0
54	MG	2A	3614	1/1	0.93	0.34	47,47,47,47	0
54	MG	2A	3072	1/1	0.93	0.35	52,52,52,52	0
54	MG	2A	3344	1/1	0.93	0.13	35,35,35,35	0
54	MG	1A	3600	1/1	0.93	0.15	41,41,41,41	0
54	MG	10	104	1/1	0.93	0.08	44,44,44,44	0
54	MG	2A	3081	1/1	0.93	0.13	47,47,47,47	0
54	MG	1A	3974	1/1	0.93	0.15	60,60,60,60	0
54	MG	2A	3350	1/1	0.93	0.12	50,50,50,50	0
54	MG	2A	3085	1/1	0.93	0.14	54,54,54,54	0
54	MG	2A	3629	1/1	0.93	0.20	43,43,43,43	0
54	MG	2a	3081	1/1	0.93	0.09	60,60,60,60	0
54	MG	2a	3083	1/1	0.93	0.10	48,48,48,48	0
54	MG	2A	3353	1/1	0.93	0.12	69,69,69,69	0
54	MG	2a	3088	1/1	0.93	0.24	50,50,50,50	0
54	MG	10	107	1/1	0.93	0.11	45,45,45,45	0
54	MG	2A	3088	1/1	0.93	0.30	34,34,34,34	0
54	MG	1a	3157	1/1	0.93	0.15	46,46,46,46	0
54	MG	1a	3159	1/1	0.93	0.08	64,64,64,64	0
54	MG	1A	3975	1/1	0.93	0.09	50,50,50,50	0
54	MG	2A	3093	1/1	0.93	0.23	64,64,64,64	0
54	MG	1A	3110	1/1	0.93	0.54	27,27,27,27	0
54	MG	1a	3163	1/1	0.93	0.27	59,59,59,59	0
54	MG	1a	3164	1/1	0.93	0.13	39,39,39,39	0
54	MG	2a	3100	1/1	0.93	0.23	80,80,80,80	0
54	MG	11	105	1/1	0.93	0.11	46,46,46,46	0
54	MG	2A	3383	1/1	0.93	0.06	38,38,38,38	0
54	MG	2A	3099	1/1	0.93	0.14	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3119	1/1	0.93	0.21	43,43,43,43	0
54	MG	1A	3494	1/1	0.93	0.14	25,25,25,25	0
54	MG	13	104	1/1	0.93	0.07	46,46,46,46	0
54	MG	2A	3106	1/1	0.93	0.08	37,37,37,37	0
54	MG	2A	3107	1/1	0.93	0.15	58,58,58,58	0
54	MG	1a	3174	1/1	0.93	0.17	60,60,60,60	0
54	MG	1A	3826	1/1	0.93	0.16	39,39,39,39	0
54	MG	1A	3832	1/1	0.93	0.17	54,54,54,54	0
54	MG	15	101	1/1	0.93	0.44	34,34,34,34	0
54	MG	1A	3835	1/1	0.93	0.64	36,36,36,36	0
54	MG	1A	3840	1/1	0.93	0.10	21,21,21,21	0
54	MG	1a	3184	1/1	0.93	0.17	63,63,63,63	0
54	MG	2A	3670	1/1	0.93	0.05	57,57,57,57	0
54	MG	1a	3186	1/1	0.93	0.08	64,64,64,64	0
54	MG	1A	3151	1/1	0.93	0.14	36,36,36,36	0
54	MG	1A	3722	1/1	0.93	0.38	47,47,47,47	0
54	MG	17	102	1/1	0.93	0.29	32,32,32,32	0
54	MG	2A	3419	1/1	0.93	0.13	37,37,37,37	0
54	MG	1A	3991	1/1	0.93	0.22	43,43,43,43	0
54	MG	1A	3008	1/1	0.93	0.16	31,31,31,31	0
54	MG	1A	3409	1/1	0.93	0.16	18,18,18,18	0
54	MG	2A	3144	1/1	0.93	0.10	41,41,41,41	0
54	MG	1A	3848	1/1	0.93	0.16	33,33,33,33	0
54	MG	1A	3122	1/1	0.93	0.27	33,33,33,33	0
54	MG	2a	3145	1/1	0.93	0.06	56,56,56,56	0
54	MG	1A	3338	1/1	0.93	0.18	21,21,21,21	0
54	MG	2A	3149	1/1	0.93	0.12	48,48,48,48	0
54	MG	1A	3222	1/1	0.93	0.71	33,33,33,33	0
54	MG	1A	4002	1/1	0.93	0.07	40,40,40,40	0
54	MG	1a	3006	1/1	0.93	0.15	57,57,57,57	0
54	MG	2A	3155	1/1	0.93	0.19	46,46,46,46	0
54	MG	1A	3341	1/1	0.93	0.15	37,37,37,37	0
54	MG	2a	3155	1/1	0.93	0.05	64,64,64,64	0
54	MG	2a	3156	1/1	0.93	0.12	45,45,45,45	0
54	MG	1A	3279	1/1	0.93	0.59	48,48,48,48	0
54	MG	1A	3077	1/1	0.93	0.26	22,22,22,22	0
54	MG	1a	3012	1/1	0.93	0.19	24,24,24,24	0
54	MG	2A	3166	1/1	0.93	0.43	40,40,40,40	0
54	MG	2A	3705	1/1	0.93	0.19	39,39,39,39	0
54	MG	2A	3707	1/1	0.93	0.39	52,52,52,52	0
54	MG	1A	3420	1/1	0.93	0.16	19,19,19,19	0
54	MG	1A	4010	1/1	0.93	0.60	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3510	1/1	0.93	0.19	16,16,16,16	0
54	MG	2a	3172	1/1	0.93	0.26	68,68,68,68	0
54	MG	2a	3173	1/1	0.93	0.15	47,47,47,47	0
54	MG	1A	3514	1/1	0.93	0.17	13,13,13,13	0
54	MG	1A	3285	1/1	0.93	0.53	39,39,39,39	0
54	MG	2a	3179	1/1	0.93	0.06	59,59,59,59	0
54	MG	1a	3222	1/1	0.93	0.19	51,51,51,51	0
54	MG	1a	3223	1/1	0.93	0.07	55,55,55,55	0
54	MG	2A	3722	1/1	0.93	0.07	48,48,48,48	0
54	MG	1A	4020	1/1	0.93	0.16	53,53,53,53	0
54	MG	1A	3872	1/1	0.93	0.09	72,72,72,72	0
54	MG	1a	3023	1/1	0.93	0.17	64,64,64,64	0
54	MG	1A	4022	1/1	0.93	0.20	51,51,51,51	0
54	MG	2a	3189	1/1	0.93	0.05	64,64,64,64	0
54	MG	1a	3026	1/1	0.93	0.20	50,50,50,50	0
54	MG	1a	3235	1/1	0.93	0.06	57,57,57,57	0
54	MG	1A	3125	1/1	0.93	0.03	65,65,65,65	0
54	MG	1a	3239	1/1	0.93	0.55	47,47,47,47	0
54	MG	1A	3520	1/1	0.93	0.12	31,31,31,31	0
54	MG	2A	3465	1/1	0.93	0.11	60,60,60,60	0
54	MG	1A	3877	1/1	0.93	0.06	38,38,38,38	0
54	MG	1a	3243	1/1	0.93	0.21	51,51,51,51	0
54	MG	2A	3470	1/1	0.93	0.12	36,36,36,36	0
54	MG	2A	3197	1/1	0.93	0.30	60,60,60,60	0
54	MG	1A	4028	1/1	0.93	0.11	29,29,29,29	0
54	MG	1A	3035	1/1	0.93	0.21	41,41,41,41	0
54	MG	1A	3236	1/1	0.93	0.38	25,25,25,25	0
54	MG	1A	3009	1/1	0.93	0.35	25,25,25,25	0
54	MG	1A	3196	1/1	0.93	0.36	28,28,28,28	0
54	MG	2A	3203	1/1	0.93	0.42	59,59,59,59	0
54	MG	1a	3038	1/1	0.93	0.21	63,63,63,63	0
54	MG	1a	3254	1/1	0.93	0.09	49,49,49,49	0
54	MG	1A	3884	1/1	0.93	0.09	56,56,56,56	0
54	MG	1A	3061	1/1	0.94	0.34	40,40,40,40	0
54	MG	1A	3505	1/1	0.94	0.16	16,16,16,16	0
54	MG	1A	3616	1/1	0.94	0.14	38,38,38,38	0
54	MG	2A	3178	1/1	0.94	0.37	43,43,43,43	0
54	MG	2A	3749	1/1	0.94	0.12	53,53,53,53	0
54	MG	1a	3039	1/1	0.94	0.14	54,54,54,54	0
54	MG	1A	3016	1/1	0.94	0.62	33,33,33,33	0
54	MG	1A	3507	1/1	0.94	0.15	24,24,24,24	0
54	MG	1A	3740	1/1	0.94	0.05	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1B	203	1/1	0.94	0.33	58,58,58,58	0
54	MG	1A	3619	1/1	0.94	0.12	33,33,33,33	0
54	MG	2A	3190	1/1	0.94	0.46	47,47,47,47	0
54	MG	2A	3191	1/1	0.94	0.60	61,61,61,61	0
54	MG	1B	206	1/1	0.94	0.28	43,43,43,43	0
54	MG	1A	3888	1/1	0.94	0.13	22,22,22,22	0
54	MG	1A	3622	1/1	0.94	0.20	28,28,28,28	0
54	MG	1A	3423	1/1	0.94	0.14	21,21,21,21	0
54	MG	1A	3207	1/1	0.94	0.76	39,39,39,39	0
54	MG	1A	3150	1/1	0.94	0.72	35,35,35,35	0
54	MG	2A	3484	1/1	0.94	0.08	69,69,69,69	0
54	MG	1B	214	1/1	0.94	0.13	30,30,30,30	0
54	MG	1A	3019	1/1	0.94	0.49	22,22,22,22	0
54	MG	1a	3266	1/1	0.94	0.15	69,69,69,69	0
54	MG	1A	3631	1/1	0.94	0.34	45,45,45,45	0
54	MG	1A	3037	1/1	0.94	0.16	48,48,48,48	0
54	MG	1A	3263	1/1	0.94	0.32	34,34,34,34	0
54	MG	1A	3521	1/1	0.94	0.11	35,35,35,35	0
54	MG	1A	3914	1/1	0.94	0.11	23,23,23,23	0
54	MG	1A	3526	1/1	0.94	0.18	34,34,34,34	0
54	MG	2A	3498	1/1	0.94	0.10	38,38,38,38	0
54	MG	2D	310	1/1	0.94	0.53	41,41,41,41	0
54	MG	1A	3528	1/1	0.94	0.16	17,17,17,17	0
54	MG	1A	3639	1/1	0.94	0.13	45,45,45,45	0
54	MG	1a	3278	1/1	0.94	0.10	66,66,66,66	0
54	MG	1A	3640	1/1	0.94	0.16	46,46,46,46	0
54	MG	1A	3529	1/1	0.94	0.19	16,16,16,16	0
54	MG	1A	3924	1/1	0.94	0.07	47,47,47,47	0
54	MG	2F	302	1/1	0.94	0.11	60,60,60,60	0
54	MG	1A	3767	1/1	0.94	0.55	52,52,52,52	0
54	MG	1A	3435	1/1	0.94	0.11	50,50,50,50	0
54	MG	1A	3370	1/1	0.94	0.17	16,16,16,16	0
54	MG	1D	313	1/1	0.94	0.20	43,43,43,43	0
54	MG	2A	3221	1/1	0.94	0.11	50,50,50,50	0
54	MG	1A	3929	1/1	0.94	0.13	22,22,22,22	0
54	MG	1A	3646	1/1	0.94	0.12	21,21,21,21	0
54	MG	1E	303	1/1	0.94	0.08	27,27,27,27	0
54	MG	1a	3087	1/1	0.94	0.12	48,48,48,48	0
54	MG	1A	3647	1/1	0.94	0.10	51,51,51,51	0
54	MG	1i	201	1/1	0.94	0.17	56,56,56,56	0
54	MG	2A	3521	1/1	0.94	0.19	53,53,53,53	0
54	MG	1a	3089	1/1	0.94	0.14	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3532	1/1	0.94	0.30	51,51,51,51	0
54	MG	2V	203	1/1	0.94	0.09	54,54,54,54	0
54	MG	1A	3371	1/1	0.94	0.15	27,27,27,27	0
54	MG	1F	305	1/1	0.94	0.47	25,25,25,25	0
54	MG	20	101	1/1	0.94	0.46	41,41,41,41	0
54	MG	1F	308	1/1	0.94	0.36	19,19,19,19	0
54	MG	1o	102	1/1	0.94	0.21	48,48,48,48	0
54	MG	1F	310	1/1	0.94	0.20	45,45,45,45	0
54	MG	2A	3531	1/1	0.94	0.14	51,51,51,51	0
54	MG	23	102	1/1	0.94	0.12	35,35,35,35	0
54	MG	1F	312	1/1	0.94	0.83	39,39,39,39	0
54	MG	1A	3780	1/1	0.94	0.16	42,42,42,42	0
54	MG	1A	3058	1/1	0.94	0.09	39,39,39,39	0
54	MG	1A	3535	1/1	0.94	0.07	40,40,40,40	0
54	MG	1A	3941	1/1	0.94	0.10	38,38,38,38	0
54	MG	2A	3248	1/1	0.94	0.76	40,40,40,40	0
54	MG	2A	3540	1/1	0.94	0.12	75,75,75,75	0
54	MG	2A	3541	1/1	0.94	0.10	33,33,33,33	0
54	MG	1A	3785	1/1	0.94	0.15	20,20,20,20	0
54	MG	2A	3005	1/1	0.94	0.10	51,51,51,51	0
54	MG	2A	3251	1/1	0.94	0.86	41,41,41,41	0
54	MG	1A	3786	1/1	0.94	0.13	27,27,27,27	0
54	MG	2a	3012	1/1	0.94	0.13	49,49,49,49	0
54	MG	1A	3440	1/1	0.94	0.21	48,48,48,48	0
54	MG	2A	3256	1/1	0.94	0.06	61,61,61,61	0
54	MG	2A	3011	1/1	0.94	0.19	25,25,25,25	0
54	MG	1a	3110	1/1	0.94	0.14	20,20,20,20	0
54	MG	2a	3020	1/1	0.94	0.16	72,72,72,72	0
54	MG	2A	3013	1/1	0.94	0.13	24,24,24,24	0
54	MG	2a	3022	1/1	0.94	0.11	52,52,52,52	0
54	MG	1a	3111	1/1	0.94	0.19	29,29,29,29	0
54	MG	1H	202	1/1	0.94	0.14	38,38,38,38	0
54	MG	1N	201	1/1	0.94	0.21	40,40,40,40	0
54	MG	1A	3656	1/1	0.94	0.56	32,32,32,32	0
54	MG	1O	201	1/1	0.94	0.34	43,43,43,43	0
54	MG	1A	3441	1/1	0.94	0.21	35,35,35,35	0
54	MG	2A	3027	1/1	0.94	0.19	46,46,46,46	0
54	MG	1A	3138	1/1	0.94	0.12	34,34,34,34	0
54	MG	1A	3952	1/1	0.94	0.18	34,34,34,34	0
54	MG	2a	3034	1/1	0.94	0.20	52,52,52,52	0
54	MG	2A	3032	1/1	0.94	0.12	28,28,28,28	0
54	MG	1A	3660	1/1	0.94	0.41	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3282	1/1	0.94	0.12	49,49,49,49	0
54	MG	1Q	203	1/1	0.94	0.09	26,26,26,26	0
54	MG	1A	3792	1/1	0.94	0.16	38,38,38,38	0
54	MG	1A	3956	1/1	0.94	0.07	50,50,50,50	0
54	MG	2A	3287	1/1	0.94	0.13	33,33,33,33	0
54	MG	2A	3038	1/1	0.94	0.12	50,50,50,50	0
54	MG	1A	3661	1/1	0.94	0.14	45,45,45,45	0
54	MG	1A	3959	1/1	0.94	0.15	42,42,42,42	0
54	MG	1S	201	1/1	0.94	0.10	54,54,54,54	0
54	MG	2A	3044	1/1	0.94	0.30	27,27,27,27	0
54	MG	2A	3296	1/1	0.94	0.12	40,40,40,40	0
54	MG	2A	3297	1/1	0.94	0.07	38,38,38,38	0
54	MG	1A	3158	1/1	0.94	0.83	29,29,29,29	0
54	MG	1A	3269	1/1	0.94	0.26	39,39,39,39	0
54	MG	2A	3300	1/1	0.94	0.23	71,71,71,71	0
54	MG	1a	3139	1/1	0.94	0.13	47,47,47,47	0
54	MG	1A	3324	1/1	0.94	0.37	53,53,53,53	0
54	MG	2A	3594	1/1	0.94	0.22	49,49,49,49	0
54	MG	1a	3142	1/1	0.94	0.09	57,57,57,57	0
54	MG	1U	204	1/1	0.94	0.76	33,33,33,33	0
54	MG	1A	3966	1/1	0.94	0.13	17,17,17,17	0
54	MG	1U	208	1/1	0.94	0.41	36,36,36,36	0
54	MG	2A	3312	1/1	0.94	0.12	42,42,42,42	0
54	MG	2a	3067	1/1	0.94	0.08	52,52,52,52	0
54	MG	1A	3186	1/1	0.94	0.21	48,48,48,48	0
54	MG	1W	203	1/1	0.94	0.28	26,26,26,26	0
54	MG	2A	3319	1/1	0.94	0.18	50,50,50,50	0
54	MG	2A	3604	1/1	0.94	0.12	30,30,30,30	0
54	MG	2A	3320	1/1	0.94	0.18	38,38,38,38	0
54	MG	2A	3061	1/1	0.94	0.65	43,43,43,43	0
54	MG	2A	3062	1/1	0.94	0.25	41,41,41,41	0
54	MG	1A	3675	1/1	0.94	0.25	46,46,46,46	0
54	MG	1A	3558	1/1	0.94	0.09	12,12,12,12	0
54	MG	1A	3677	1/1	0.94	0.10	36,36,36,36	0
54	MG	2A	3066	1/1	0.94	0.82	52,52,52,52	0
54	MG	2a	3082	1/1	0.94	0.14	68,68,68,68	0
54	MG	1A	3678	1/1	0.94	0.24	14,14,14,14	0
54	MG	2a	3085	1/1	0.94	0.09	53,53,53,53	0
54	MG	1A	3560	1/1	0.94	0.17	35,35,35,35	0
54	MG	1a	3160	1/1	0.94	0.15	48,48,48,48	0
54	MG	1A	3451	1/1	0.94	0.14	51,51,51,51	0
54	MG	1A	3273	1/1	0.94	0.15	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3682	1/1	0.94	0.07	33,33,33,33	0
54	MG	1A	3117	1/1	0.94	0.18	24,24,24,24	0
54	MG	2A	3075	1/1	0.94	0.17	24,24,24,24	0
54	MG	2A	3076	1/1	0.94	0.51	44,44,44,44	0
54	MG	2A	3079	1/1	0.94	0.91	54,54,54,54	0
54	MG	1A	3012	1/1	0.94	0.10	33,33,33,33	0
54	MG	1A	3332	1/1	0.94	0.18	46,46,46,46	0
54	MG	2A	3082	1/1	0.94	1.17	56,56,56,56	0
54	MG	1a	3170	1/1	0.94	0.19	64,64,64,64	0
54	MG	1A	3467	1/1	0.94	0.17	19,19,19,19	0
54	MG	1A	3689	1/1	0.94	0.63	31,31,31,31	0
54	MG	1A	3817	1/1	0.94	0.11	38,38,38,38	0
54	MG	1A	3470	1/1	0.94	0.10	49,49,49,49	0
54	MG	2A	3359	1/1	0.94	0.16	26,26,26,26	0
54	MG	2A	3645	1/1	0.94	0.31	48,48,48,48	0
54	MG	2A	3360	1/1	0.94	0.14	39,39,39,39	0
54	MG	1A	3277	1/1	0.94	0.22	27,27,27,27	0
54	MG	2a	3112	1/1	0.94	0.08	47,47,47,47	0
54	MG	2A	3649	1/1	0.94	0.11	47,47,47,47	0
54	MG	2a	3114	1/1	0.94	0.10	51,51,51,51	0
54	MG	1A	3822	1/1	0.94	0.16	54,54,54,54	0
54	MG	2A	3365	1/1	0.94	0.12	48,48,48,48	0
54	MG	2A	3653	1/1	0.94	0.07	55,55,55,55	0
54	MG	2A	3366	1/1	0.94	0.18	42,42,42,42	0
54	MG	1A	3473	1/1	0.94	0.17	44,44,44,44	0
54	MG	2A	3094	1/1	0.94	0.18	35,35,35,35	0
54	MG	1A	3163	1/1	0.94	0.18	45,45,45,45	0
54	MG	1a	3183	1/1	0.94	0.08	65,65,65,65	0
54	MG	2a	3127	1/1	0.94	0.09	57,57,57,57	0
54	MG	2A	3663	1/1	0.94	0.11	45,45,45,45	0
54	MG	1A	3399	1/1	0.94	0.11	42,42,42,42	0
54	MG	1a	3185	1/1	0.94	0.14	44,44,44,44	0
54	MG	1A	3053	1/1	0.94	0.54	24,24,24,24	0
54	MG	1A	3478	1/1	0.94	0.08	61,61,61,61	0
54	MG	2A	3388	1/1	0.94	0.10	49,49,49,49	0
54	MG	1A	3837	1/1	0.94	0.24	26,26,26,26	0
54	MG	2A	3103	1/1	0.94	0.09	49,49,49,49	0
54	MG	1A	3404	1/1	0.94	0.15	20,20,20,20	0
54	MG	2A	3672	1/1	0.94	0.09	35,35,35,35	0
54	MG	1A	3702	1/1	0.94	0.08	44,44,44,44	0
54	MG	2a	3147	1/1	0.94	0.29	69,69,69,69	0
54	MG	1A	3589	1/1	0.94	0.33	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3108	1/1	0.94	0.21	46,46,46,46	0
54	MG	2A	3111	1/1	0.94	0.52	41,41,41,41	0
54	MG	1a	3193	1/1	0.94	0.20	72,72,72,72	0
54	MG	1A	3705	1/1	0.94	0.20	52,52,52,52	0
54	MG	2A	3115	1/1	0.94	0.17	69,69,69,69	0
54	MG	1A	3226	1/1	0.94	0.61	28,28,28,28	0
54	MG	1a	3197	1/1	0.94	0.26	60,60,60,60	0
54	MG	2A	3684	1/1	0.94	0.06	42,42,42,42	0
54	MG	2A	3120	1/1	0.94	0.20	46,46,46,46	0
54	MG	2A	3410	1/1	0.94	0.16	31,31,31,31	0
54	MG	1A	4008	1/1	0.94	0.07	55,55,55,55	0
54	MG	1A	3846	1/1	0.94	0.12	39,39,39,39	0
54	MG	2A	3416	1/1	0.94	0.10	38,38,38,38	0
54	MG	2A	3128	1/1	0.94	0.70	42,42,42,42	0
54	MG	1A	3229	1/1	0.94	0.14	40,40,40,40	0
54	MG	1A	3709	1/1	0.94	0.09	47,47,47,47	0
54	MG	1a	3202	1/1	0.94	0.30	70,70,70,70	0
54	MG	1A	3407	1/1	0.94	0.17	22,22,22,22	0
54	MG	2A	3698	1/1	0.94	0.07	58,58,58,58	0
54	MG	1A	3712	1/1	0.94	0.18	39,39,39,39	0
54	MG	2a	3176	1/1	0.94	0.13	63,63,63,63	0
54	MG	2a	3178	1/1	0.94	0.07	47,47,47,47	0
54	MG	1A	3713	1/1	0.94	0.38	24,24,24,24	0
54	MG	2A	3704	1/1	0.94	0.09	55,55,55,55	0
54	MG	1A	3168	1/1	0.94	0.17	36,36,36,36	0
54	MG	2A	3141	1/1	0.94	0.47	43,43,43,43	0
54	MG	1a	3016	1/1	0.94	0.10	68,68,68,68	0
54	MG	1A	3715	1/1	0.94	0.39	48,48,48,48	0
54	MG	1a	3213	1/1	0.94	0.22	54,54,54,54	0
54	MG	2a	3186	1/1	0.94	0.06	58,58,58,58	0
54	MG	1A	3088	1/1	0.94	0.34	32,32,32,32	0
54	MG	1A	4025	1/1	0.94	0.41	30,30,30,30	0
54	MG	1A	3862	1/1	0.94	0.09	36,36,36,36	0
54	MG	2a	3193	1/1	0.94	0.07	52,52,52,52	0
54	MG	1A	3288	1/1	0.94	0.13	32,32,32,32	0
54	MG	1a	3221	1/1	0.94	0.12	35,35,35,35	0
54	MG	1A	3199	1/1	0.94	0.17	33,33,33,33	0
54	MG	2A	3442	1/1	0.94	0.20	38,38,38,38	0
54	MG	2a	3199	1/1	0.94	0.08	73,73,73,73	0
54	MG	2e	201	1/1	0.94	0.26	63,63,63,63	0
54	MG	1A	3870	1/1	0.94	0.15	38,38,38,38	0
54	MG	2A	3727	1/1	0.94	0.56	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3290	1/1	0.94	0.28	43,43,43,43	0
54	MG	1A	3175	1/1	0.94	0.40	31,31,31,31	0
54	MG	1A	3416	1/1	0.94	0.21	10,10,10,10	0
56	MPD	1a	3280	8/8	0.94	0.24	47,64,65,66	0
54	MG	2A	3163	1/1	0.94	0.11	68,68,68,68	0
54	MG	1a	3228	1/1	0.94	0.31	75,75,75,75	0
54	MG	1a	3231	1/1	0.94	0.21	43,43,43,43	0
54	MG	1a	3030	1/1	0.94	0.13	47,47,47,47	0
54	MG	2A	3453	1/1	0.94	0.24	54,54,54,54	0
54	MG	1A	3201	1/1	0.94	0.51	39,39,39,39	0
54	MG	1A	4037	1/1	0.94	0.18	26,26,26,26	0
54	MG	1a	3237	1/1	0.94	0.09	62,62,62,62	0
54	MG	1A	3355	1/1	0.94	0.09	28,28,28,28	0
54	MG	15	102	1/1	0.95	0.78	31,31,31,31	0
54	MG	1A	3005	1/1	0.95	0.17	19,19,19,19	0
54	MG	2A	3039	1/1	0.95	0.16	66,66,66,66	0
54	MG	1A	3784	1/1	0.95	0.12	45,45,45,45	0
54	MG	2B	210	1/1	0.95	0.20	56,56,56,56	0
54	MG	15	106	1/1	0.95	0.11	41,41,41,41	0
54	MG	2A	3253	1/1	0.95	0.20	52,52,52,52	0
54	MG	1A	3316	1/1	0.95	0.29	31,31,31,31	0
54	MG	1A	3086	1/1	0.95	0.23	56,56,56,56	0
54	MG	1A	3318	1/1	0.95	0.20	36,36,36,36	0
54	MG	1A	3265	1/1	0.95	0.15	40,40,40,40	0
54	MG	1A	3601	1/1	0.95	0.06	33,33,33,33	0
54	MG	1a	3169	1/1	0.95	0.10	44,44,44,44	0
54	MG	18	101	1/1	0.95	0.24	25,25,25,25	0
54	MG	1A	4038	1/1	0.95	0.05	51,51,51,51	0
54	MG	2D	307	1/1	0.95	0.45	63,63,63,63	0
54	MG	2D	308	1/1	0.95	0.33	55,55,55,55	0
54	MG	1A	3602	1/1	0.95	0.09	44,44,44,44	0
54	MG	1A	3128	1/1	0.95	0.25	27,27,27,27	0
54	MG	2A	3266	1/1	0.95	0.63	35,35,35,35	0
54	MG	1A	4041	1/1	0.95	0.12	41,41,41,41	0
54	MG	2A	3522	1/1	0.95	0.46	59,59,59,59	0
54	MG	2E	302	1/1	0.95	0.11	36,36,36,36	0
54	MG	2A	3523	1/1	0.95	0.07	38,38,38,38	0
54	MG	1A	3919	1/1	0.95	0.13	44,44,44,44	0
54	MG	2A	3272	1/1	0.95	0.10	26,26,26,26	0
54	MG	1A	3129	1/1	0.95	0.39	27,27,27,27	0
54	MG	1A	4046	1/1	0.95	0.11	56,56,56,56	0
54	MG	2A	3276	1/1	0.95	0.08	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1a	3181	1/1	0.95	0.13	60,60,60,60	0
54	MG	1A	4047	1/1	0.95	0.10	46,46,46,46	0
54	MG	1A	3374	1/1	0.95	0.14	21,21,21,21	0
54	MG	2A	3281	1/1	0.95	0.24	60,60,60,60	0
54	MG	2A	3533	1/1	0.95	0.18	65,65,65,65	0
54	MG	1A	3512	1/1	0.95	0.18	35,35,35,35	0
54	MG	1B	201	1/1	0.95	0.15	59,59,59,59	0
54	MG	1A	3197	1/1	0.95	0.38	49,49,49,49	0
54	MG	1A	3926	1/1	0.95	0.14	29,29,29,29	0
54	MG	1B	204	1/1	0.95	0.10	40,40,40,40	0
54	MG	2R	203	1/1	0.95	0.15	19,19,19,19	0
54	MG	1A	3798	1/1	0.95	0.28	27,27,27,27	0
54	MG	2T	202	1/1	0.95	0.09	45,45,45,45	0
54	MG	2T	203	1/1	0.95	0.10	46,46,46,46	0
54	MG	1A	3132	1/1	0.95	0.12	29,29,29,29	0
54	MG	1A	3696	1/1	0.95	0.10	49,49,49,49	0
54	MG	2A	3292	1/1	0.95	0.08	25,25,25,25	0
54	MG	1A	3044	1/1	0.95	0.19	22,22,22,22	0
54	MG	2A	3294	1/1	0.95	0.13	24,24,24,24	0
54	MG	1A	3519	1/1	0.95	0.30	32,32,32,32	0
54	MG	1A	3933	1/1	0.95	0.39	26,26,26,26	0
54	MG	1A	3325	1/1	0.95	0.10	47,47,47,47	0
54	MG	1A	3935	1/1	0.95	0.14	37,37,37,37	0
54	MG	2A	3553	1/1	0.95	0.12	47,47,47,47	0
54	MG	1A	3179	1/1	0.95	0.35	27,27,27,27	0
54	MG	2A	3555	1/1	0.95	0.07	47,47,47,47	0
54	MG	1A	3234	1/1	0.95	0.33	33,33,33,33	0
54	MG	2A	3084	1/1	0.95	0.10	67,67,67,67	0
54	MG	2A	3304	1/1	0.95	0.16	52,52,52,52	0
54	MG	1A	3938	1/1	0.95	0.07	52,52,52,52	0
54	MG	1B	219	1/1	0.95	0.10	33,33,33,33	0
54	MG	1A	3527	1/1	0.95	0.19	13,13,13,13	0
54	MG	1A	3202	1/1	0.95	0.37	47,47,47,47	0
54	MG	1a	3033	1/1	0.95	0.13	26,26,26,26	0
54	MG	2A	3091	1/1	0.95	0.31	31,31,31,31	0
54	MG	1B	223	1/1	0.95	0.17	47,47,47,47	0
54	MG	2A	3317	1/1	0.95	0.15	53,53,53,53	0
54	MG	2a	3013	1/1	0.95	0.08	50,50,50,50	0
54	MG	1A	3621	1/1	0.95	0.11	39,39,39,39	0
54	MG	1A	3811	1/1	0.95	0.13	54,54,54,54	0
54	MG	1A	3944	1/1	0.95	0.08	37,37,37,37	0
54	MG	1A	3330	1/1	0.95	0.12	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1a	3216	1/1	0.95	0.08	58,58,58,58	0
54	MG	1D	302	1/1	0.95	0.47	23,23,23,23	0
54	MG	1A	3237	1/1	0.95	0.42	22,22,22,22	0
54	MG	1A	3454	1/1	0.95	0.16	48,48,48,48	0
54	MG	2A	3330	1/1	0.95	0.15	35,35,35,35	0
54	MG	2A	3331	1/1	0.95	0.14	42,42,42,42	0
54	MG	1A	3455	1/1	0.95	0.16	16,16,16,16	0
54	MG	2a	3027	1/1	0.95	0.13	64,64,64,64	0
54	MG	2A	3333	1/1	0.95	0.20	50,50,50,50	0
54	MG	2A	3585	1/1	0.95	0.19	46,46,46,46	0
54	MG	1D	307	1/1	0.95	0.17	10,10,10,10	0
54	MG	1A	3154	1/1	0.95	0.48	35,35,35,35	0
54	MG	1A	3064	1/1	0.95	0.09	42,42,42,42	0
54	MG	1A	3045	1/1	0.95	0.15	33,33,33,33	0
54	MG	1D	312	1/1	0.95	0.15	32,32,32,32	0
54	MG	1a	3227	1/1	0.95	0.08	43,43,43,43	0
54	MG	2a	3037	1/1	0.95	0.15	55,55,55,55	0
54	MG	1A	3465	1/1	0.95	0.10	35,35,35,35	0
54	MG	1a	3229	1/1	0.95	0.09	65,65,65,65	0
54	MG	2A	3345	1/1	0.95	0.17	50,50,50,50	0
54	MG	1a	3230	1/1	0.95	0.10	48,48,48,48	0
54	MG	1D	314	1/1	0.95	0.14	44,44,44,44	0
54	MG	1D	315	1/1	0.95	0.20	44,44,44,44	0
54	MG	1A	3955	1/1	0.95	0.09	47,47,47,47	0
54	MG	1a	3059	1/1	0.95	0.45	48,48,48,48	0
54	MG	2A	3124	1/1	0.95	0.39	33,33,33,33	0
54	MG	1A	3403	1/1	0.95	0.15	15,15,15,15	0
54	MG	1A	3542	1/1	0.95	0.09	34,34,34,34	0
54	MG	1A	3241	1/1	0.95	0.59	36,36,36,36	0
54	MG	2A	3610	1/1	0.95	0.07	42,42,42,42	0
54	MG	1a	3064	1/1	0.95	0.53	71,71,71,71	0
54	MG	1a	3241	1/1	0.95	0.11	56,56,56,56	0
54	MG	1E	306	1/1	0.95	0.10	39,39,39,39	0
54	MG	1A	3548	1/1	0.95	0.12	43,43,43,43	0
54	MG	2A	3615	1/1	0.95	0.07	39,39,39,39	0
54	MG	2A	3616	1/1	0.95	0.13	59,59,59,59	0
54	MG	1A	3830	1/1	0.95	0.07	44,44,44,44	0
54	MG	2A	3363	1/1	0.95	0.21	37,37,37,37	0
54	MG	2A	3619	1/1	0.95	0.13	30,30,30,30	0
54	MG	1A	3471	1/1	0.95	0.06	35,35,35,35	0
54	MG	1a	3069	1/1	0.95	0.15	40,40,40,40	0
54	MG	1A	3337	1/1	0.95	0.14	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3369	1/1	0.95	0.11	44,44,44,44	0
54	MG	1a	3250	1/1	0.95	0.10	37,37,37,37	0
54	MG	2A	3372	1/1	0.95	0.09	27,27,27,27	0
54	MG	2A	3373	1/1	0.95	0.18	53,53,53,53	0
54	MG	2A	3374	1/1	0.95	0.15	36,36,36,36	0
54	MG	1A	3554	1/1	0.95	0.07	44,44,44,44	0
54	MG	2A	3378	1/1	0.95	0.07	73,73,73,73	0
54	MG	1F	311	1/1	0.95	0.21	28,28,28,28	0
54	MG	1A	3839	1/1	0.95	0.11	52,52,52,52	0
54	MG	1a	3255	1/1	0.95	0.14	43,43,43,43	0
54	MG	2A	3637	1/1	0.95	0.13	52,52,52,52	0
54	MG	1A	3243	1/1	0.95	0.66	60,60,60,60	0
54	MG	1A	3735	1/1	0.95	0.17	23,23,23,23	0
54	MG	2A	3641	1/1	0.95	0.11	74,74,74,74	0
54	MG	2A	3386	1/1	0.95	0.09	47,47,47,47	0
54	MG	2A	3152	1/1	0.95	0.17	55,55,55,55	0
54	MG	1A	3245	1/1	0.95	0.17	32,32,32,32	0
54	MG	1a	3260	1/1	0.95	0.07	56,56,56,56	0
54	MG	2a	3093	1/1	0.95	0.11	60,60,60,60	0
54	MG	2A	3156	1/1	0.95	0.28	48,48,48,48	0
54	MG	1A	3738	1/1	0.95	0.18	23,23,23,23	0
54	MG	1A	3046	1/1	0.95	0.12	34,34,34,34	0
54	MG	1A	3184	1/1	0.95	0.08	43,43,43,43	0
54	MG	2A	3395	1/1	0.95	0.19	35,35,35,35	0
54	MG	2A	3397	1/1	0.95	0.23	40,40,40,40	0
54	MG	1A	3410	1/1	0.95	0.17	17,17,17,17	0
54	MG	2A	3164	1/1	0.95	0.49	45,45,45,45	0
54	MG	1A	3293	1/1	0.95	0.49	44,44,44,44	0
54	MG	2A	3659	1/1	0.95	0.06	51,51,51,51	0
54	MG	1A	3744	1/1	0.95	0.15	29,29,29,29	0
54	MG	1N	202	1/1	0.95	0.32	40,40,40,40	0
54	MG	1N	203	1/1	0.95	0.17	58,58,58,58	0
54	MG	2A	3407	1/1	0.95	0.14	23,23,23,23	0
54	MG	1A	3481	1/1	0.95	0.07	46,46,46,46	0
54	MG	1A	3570	1/1	0.95	0.15	23,23,23,23	0
54	MG	2A	3411	1/1	0.95	0.15	54,54,54,54	0
54	MG	1P	201	1/1	0.95	0.69	34,34,34,34	0
54	MG	1A	3854	1/1	0.95	0.12	31,31,31,31	0
54	MG	2a	3115	1/1	0.95	0.11	72,72,72,72	0
54	MG	2a	3116	1/1	0.95	0.10	73,73,73,73	0
54	MG	1a	3277	1/1	0.95	0.25	65,65,65,65	0
54	MG	2A	3417	1/1	0.95	0.13	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3121	1/1	0.95	0.21	39,39,39,39	0
54	MG	2A	3176	1/1	0.95	0.09	33,33,33,33	0
54	MG	1a	3096	1/1	0.95	0.18	43,43,43,43	0
54	MG	1A	3856	1/1	0.95	0.13	37,37,37,37	0
54	MG	2A	3181	1/1	0.95	0.14	45,45,45,45	0
54	MG	1A	3486	1/1	0.95	0.12	20,20,20,20	0
54	MG	1A	3750	1/1	0.95	0.21	28,28,28,28	0
54	MG	1R	201	1/1	0.95	0.32	26,26,26,26	0
54	MG	1A	3487	1/1	0.95	0.07	28,28,28,28	0
54	MG	2a	3130	1/1	0.95	0.22	61,61,61,61	0
54	MG	1a	3106	1/1	0.95	0.13	44,44,44,44	0
54	MG	1A	3993	1/1	0.95	0.15	18,18,18,18	0
54	MG	1A	3298	1/1	0.95	0.11	29,29,29,29	0
54	MG	2a	3137	1/1	0.95	0.09	46,46,46,46	0
54	MG	1f	202	1/1	0.95	0.20	36,36,36,36	0
54	MG	1A	3996	1/1	0.95	0.14	44,44,44,44	0
54	MG	1A	3023	1/1	0.95	0.17	22,22,22,22	0
54	MG	2a	3143	1/1	0.95	0.11	57,57,57,57	0
54	MG	1a	3112	1/1	0.95	0.06	69,69,69,69	0
54	MG	1A	3579	1/1	0.95	0.12	48,48,48,48	0
54	MG	1T	205	1/1	0.95	0.09	59,59,59,59	0
54	MG	2A	3693	1/1	0.95	0.12	38,38,38,38	0
54	MG	2A	3694	1/1	0.95	0.08	29,29,29,29	0
54	MG	1A	3663	1/1	0.95	0.14	29,29,29,29	0
54	MG	2A	3696	1/1	0.95	0.11	45,45,45,45	0
54	MG	1m	201	1/1	0.95	0.09	66,66,66,66	0
54	MG	1A	3665	1/1	0.95	0.17	48,48,48,48	0
54	MG	1A	3350	1/1	0.95	0.17	19,19,19,19	0
54	MG	1A	3761	1/1	0.95	0.19	38,38,38,38	0
54	MG	1A	3668	1/1	0.95	0.33	51,51,51,51	0
54	MG	1V	204	1/1	0.95	0.17	40,40,40,40	0
54	MG	2A	3206	1/1	0.95	0.44	52,52,52,52	0
54	MG	2A	3708	1/1	0.95	0.09	49,49,49,49	0
54	MG	1A	3763	1/1	0.95	0.17	30,30,30,30	0
54	MG	2a	3164	1/1	0.95	0.13	61,61,61,61	0
54	MG	1A	4006	1/1	0.95	0.11	33,33,33,33	0
54	MG	1A	3879	1/1	0.95	0.32	31,31,31,31	0
54	MG	1a	3129	1/1	0.95	0.11	44,44,44,44	0
54	MG	2a	3169	1/1	0.95	0.15	45,45,45,45	0
54	MG	2A	3713	1/1	0.95	0.08	35,35,35,35	0
54	MG	2A	3457	1/1	0.95	0.17	51,51,51,51	0
54	MG	1a	3130	1/1	0.95	0.11	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	10	101	1/1	0.95	0.34	32,32,32,32	0
54	MG	2A	3721	1/1	0.95	0.13	42,42,42,42	0
54	MG	2A	3003	1/1	0.95	0.13	47,47,47,47	0
54	MG	1A	3669	1/1	0.95	0.13	45,45,45,45	0
54	MG	2A	3216	1/1	0.95	0.21	49,49,49,49	0
54	MG	1A	3670	1/1	0.95	0.17	40,40,40,40	0
54	MG	1a	3134	1/1	0.95	0.09	38,38,38,38	0
54	MG	1A	4011	1/1	0.95	0.16	34,34,34,34	0
54	MG	2A	3729	1/1	0.95	0.13	40,40,40,40	0
54	MG	1a	3136	1/1	0.95	0.18	54,54,54,54	0
54	MG	1A	3882	1/1	0.95	0.09	34,34,34,34	0
54	MG	2A	3014	1/1	0.95	0.46	44,44,44,44	0
54	MG	2A	3472	1/1	0.95	0.20	44,44,44,44	0
54	MG	2A	3223	1/1	0.95	0.10	48,48,48,48	0
54	MG	2A	3016	1/1	0.95	0.11	47,47,47,47	0
54	MG	1A	3768	1/1	0.95	0.17	46,46,46,46	0
54	MG	2a	3192	1/1	0.95	0.07	56,56,56,56	0
54	MG	2A	3226	1/1	0.95	0.25	62,62,62,62	0
54	MG	1l	101	1/1	0.95	0.29	36,36,36,36	0
54	MG	1A	3301	1/1	0.95	0.30	35,35,35,35	0
54	MG	2A	3741	1/1	0.95	0.08	40,40,40,40	0
54	MG	2A	3023	1/1	0.95	0.56	40,40,40,40	0
54	MG	2A	3232	1/1	0.95	0.17	50,50,50,50	0
54	MG	2a	3200	1/1	0.95	0.07	70,70,70,70	0
54	MG	1A	3582	1/1	0.95	0.22	48,48,48,48	0
54	MG	1A	3106	1/1	0.95	0.28	18,18,18,18	0
54	MG	2A	3747	1/1	0.95	0.32	54,54,54,54	0
54	MG	1A	3166	1/1	0.95	0.60	40,40,40,40	0
54	MG	1a	3146	1/1	0.95	0.12	31,31,31,31	0
56	MPD	1A	4056	8/8	0.95	0.27	39,46,54,57	0
54	MG	2A	3239	1/1	0.95	0.51	40,40,40,40	0
54	MG	2A	3751	1/1	0.95	0.27	57,57,57,57	0
54	MG	1a	3147	1/1	0.95	0.26	52,52,52,52	0
54	MG	2A	3029	1/1	0.95	0.12	28,28,28,28	0
54	MG	1A	3890	1/1	0.95	0.41	23,23,23,23	0
54	MG	2A	3493	1/1	0.95	0.12	35,35,35,35	0
54	MG	1A	3305	1/1	0.95	0.22	40,40,40,40	0
54	MG	2A	3495	1/1	0.95	0.09	39,39,39,39	0
54	MG	1A	3258	1/1	0.95	0.76	33,33,33,33	0
54	MG	1A	3262	1/1	0.95	0.65	37,37,37,37	0
54	MG	1A	3591	1/1	0.95	0.22	50,50,50,50	0
54	MG	1A	3981	1/1	0.96	0.37	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2B	216	1/1	0.96	0.12	53,53,53,53	0
54	MG	2A	3259	1/1	0.96	0.16	48,48,48,48	0
54	MG	1T	202	1/1	0.96	0.13	47,47,47,47	0
54	MG	2B	219	1/1	0.96	0.09	58,58,58,58	0
54	MG	1A	3235	1/1	0.96	0.44	29,29,29,29	0
54	MG	1a	3137	1/1	0.96	0.20	64,64,64,64	0
54	MG	1A	3983	1/1	0.96	0.17	35,35,35,35	0
54	MG	2D	305	1/1	0.96	0.24	32,32,32,32	0
54	MG	2D	306	1/1	0.96	0.45	44,44,44,44	0
54	MG	1A	3090	1/1	0.96	0.15	25,25,25,25	0
54	MG	1A	3469	1/1	0.96	0.11	37,37,37,37	0
54	MG	1U	206	1/1	0.96	0.71	33,33,33,33	0
54	MG	2A	3268	1/1	0.96	0.18	44,44,44,44	0
54	MG	1A	3043	1/1	0.96	0.15	10,10,10,10	0
54	MG	1A	3188	1/1	0.96	0.37	32,32,32,32	0
54	MG	1V	201	1/1	0.96	0.52	29,29,29,29	0
54	MG	1A	3018	1/1	0.96	0.25	23,23,23,23	0
54	MG	1A	3070	1/1	0.96	0.32	25,25,25,25	0
54	MG	1W	202	1/1	0.96	0.24	36,36,36,36	0
54	MG	2E	306	1/1	0.96	0.16	52,52,52,52	0
54	MG	1a	3150	1/1	0.96	0.11	56,56,56,56	0
54	MG	2A	3048	1/1	0.96	0.13	54,54,54,54	0
54	MG	1A	3831	1/1	0.96	0.08	39,39,39,39	0
54	MG	1A	3376	1/1	0.96	0.10	42,42,42,42	0
54	MG	1A	3833	1/1	0.96	0.24	46,46,46,46	0
54	MG	1a	3155	1/1	0.96	0.07	61,61,61,61	0
54	MG	2A	3055	1/1	0.96	0.05	41,41,41,41	0
54	MG	1A	3834	1/1	0.96	0.21	21,21,21,21	0
54	MG	2O	201	1/1	0.96	0.12	53,53,53,53	0
54	MG	1A	3475	1/1	0.96	0.10	28,28,28,28	0
54	MG	2P	201	1/1	0.96	0.09	51,51,51,51	0
54	MG	1A	3998	1/1	0.96	0.17	42,42,42,42	0
54	MG	1A	3836	1/1	0.96	0.28	28,28,28,28	0
54	MG	10	106	1/1	0.96	0.11	59,59,59,59	0
54	MG	1A	3701	1/1	0.96	0.16	20,20,20,20	0
54	MG	1A	3123	1/1	0.96	0.14	21,21,21,21	0
54	MG	1A	3703	1/1	0.96	0.06	43,43,43,43	0
54	MG	1A	3307	1/1	0.96	0.24	43,43,43,43	0
54	MG	1a	3167	1/1	0.96	0.39	56,56,56,56	0
54	MG	1A	3590	1/1	0.96	0.19	33,33,33,33	0
54	MG	13	101	1/1	0.96	0.17	26,26,26,26	0
54	MG	2V	202	1/1	0.96	0.34	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3242	1/1	0.96	0.31	32,32,32,32	0
54	MG	1A	3095	1/1	0.96	0.17	16,16,16,16	0
54	MG	2A	3302	1/1	0.96	0.10	42,42,42,42	0
54	MG	2Y	201	1/1	0.96	0.20	54,54,54,54	0
54	MG	2A	3303	1/1	0.96	0.11	49,49,49,49	0
54	MG	1A	3312	1/1	0.96	0.10	12,12,12,12	0
54	MG	1A	3313	1/1	0.96	0.43	28,28,28,28	0
54	MG	1A	3485	1/1	0.96	0.17	38,38,38,38	0
54	MG	1a	3176	1/1	0.96	0.14	45,45,45,45	0
54	MG	1A	3599	1/1	0.96	0.21	39,39,39,39	0
54	MG	27	101	1/1	0.96	0.62	38,38,38,38	0
54	MG	2A	3562	1/1	0.96	0.05	60,60,60,60	0
54	MG	1A	4012	1/1	0.96	0.62	35,35,35,35	0
54	MG	1A	3315	1/1	0.96	0.54	35,35,35,35	0
54	MG	2a	3001	1/1	0.96	0.20	31,31,31,31	0
54	MG	15	104	1/1	0.96	0.16	29,29,29,29	0
54	MG	2A	3315	1/1	0.96	0.11	45,45,45,45	0
54	MG	1A	3156	1/1	0.96	0.46	23,23,23,23	0
54	MG	1A	3853	1/1	0.96	0.20	46,46,46,46	0
54	MG	1A	4018	1/1	0.96	0.46	53,53,53,53	0
54	MG	1A	4019	1/1	0.96	0.08	54,54,54,54	0
54	MG	1A	3394	1/1	0.96	0.12	24,24,24,24	0
54	MG	1A	3717	1/1	0.96	0.40	34,34,34,34	0
54	MG	1A	3057	1/1	0.96	0.13	17,17,17,17	0
54	MG	2A	3325	1/1	0.96	0.08	35,35,35,35	0
54	MG	1A	3857	1/1	0.96	0.57	39,39,39,39	0
54	MG	1A	3492	1/1	0.96	0.16	32,32,32,32	0
54	MG	2a	3015	1/1	0.96	0.14	44,44,44,44	0
54	MG	2A	3328	1/1	0.96	0.14	33,33,33,33	0
54	MG	2A	3329	1/1	0.96	0.16	35,35,35,35	0
54	MG	1A	3002	1/1	0.96	0.17	38,38,38,38	0
54	MG	1a	3192	1/1	0.96	0.10	68,68,68,68	0
54	MG	1A	3723	1/1	0.96	0.14	54,54,54,54	0
54	MG	1A	3863	1/1	0.96	0.07	39,39,39,39	0
54	MG	1A	3724	1/1	0.96	0.09	32,32,32,32	0
54	MG	1a	3196	1/1	0.96	0.15	49,49,49,49	0
54	MG	2A	3591	1/1	0.96	0.42	65,65,65,65	0
54	MG	1A	3866	1/1	0.96	0.09	41,41,41,41	0
54	MG	1a	3005	1/1	0.96	0.10	44,44,44,44	0
54	MG	2A	3339	1/1	0.96	0.18	31,31,31,31	0
54	MG	1A	3161	1/1	0.96	0.16	40,40,40,40	0
54	MG	1A	3495	1/1	0.96	0.10	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3608	1/1	0.96	0.17	51,51,51,51	0
54	MG	1a	3009	1/1	0.96	0.16	44,44,44,44	0
54	MG	2A	3105	1/1	0.96	0.24	45,45,45,45	0
54	MG	1a	3010	1/1	0.96	0.20	47,47,47,47	0
54	MG	1A	3021	1/1	0.96	0.65	32,32,32,32	0
54	MG	1a	3205	1/1	0.96	0.11	74,74,74,74	0
54	MG	1A	3048	1/1	0.96	0.42	49,49,49,49	0
54	MG	1a	3208	1/1	0.96	0.17	53,53,53,53	0
54	MG	2A	3351	1/1	0.96	0.17	21,21,21,21	0
54	MG	1a	3209	1/1	0.96	0.12	57,57,57,57	0
54	MG	2A	3608	1/1	0.96	0.20	52,52,52,52	0
54	MG	1A	3612	1/1	0.96	0.15	32,32,32,32	0
54	MG	2a	3045	1/1	0.96	0.09	62,62,62,62	0
54	MG	1A	3613	1/1	0.96	0.09	39,39,39,39	0
54	MG	2a	3047	1/1	0.96	0.12	53,53,53,53	0
54	MG	1A	3734	1/1	0.96	0.31	33,33,33,33	0
54	MG	2A	3356	1/1	0.96	0.19	59,59,59,59	0
54	MG	1A	3252	1/1	0.96	0.49	37,37,37,37	0
54	MG	2A	3358	1/1	0.96	0.10	49,49,49,49	0
54	MG	2A	3121	1/1	0.96	0.15	38,38,38,38	0
54	MG	2a	3054	1/1	0.96	0.11	50,50,50,50	0
54	MG	2A	3122	1/1	0.96	0.43	42,42,42,42	0
54	MG	1a	3214	1/1	0.96	0.06	56,56,56,56	0
54	MG	1A	4042	1/1	0.96	0.49	40,40,40,40	0
54	MG	1A	3253	1/1	0.96	0.25	41,41,41,41	0
54	MG	2A	3364	1/1	0.96	0.26	70,70,70,70	0
54	MG	1A	3130	1/1	0.96	0.31	28,28,28,28	0
54	MG	1a	3218	1/1	0.96	0.13	54,54,54,54	0
54	MG	1A	3205	1/1	0.96	0.29	38,38,38,38	0
54	MG	1A	3022	1/1	0.96	0.22	29,29,29,29	0
54	MG	2A	3133	1/1	0.96	0.15	61,61,61,61	0
54	MG	1A	3167	1/1	0.96	0.18	31,31,31,31	0
54	MG	1A	4049	1/1	0.96	0.11	52,52,52,52	0
54	MG	1A	4050	1/1	0.96	0.11	35,35,35,35	0
54	MG	1A	3411	1/1	0.96	0.17	15,15,15,15	0
54	MG	1A	4052	1/1	0.96	0.06	45,45,45,45	0
54	MG	1A	4053	1/1	0.96	0.43	56,56,56,56	0
54	MG	2A	3143	1/1	0.96	0.32	42,42,42,42	0
54	MG	2A	3382	1/1	0.96	0.11	48,48,48,48	0
54	MG	1A	4054	1/1	0.96	0.12	34,34,34,34	0
54	MG	2A	3145	1/1	0.96	0.09	28,28,28,28	0
54	MG	1A	3208	1/1	0.96	0.32	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3133	1/1	0.96	0.39	21,21,21,21	0
54	MG	2A	3387	1/1	0.96	0.07	54,54,54,54	0
54	MG	1A	3889	1/1	0.96	0.13	45,45,45,45	0
54	MG	1A	3746	1/1	0.96	0.12	32,32,32,32	0
54	MG	1A	3210	1/1	0.96	0.33	29,29,29,29	0
54	MG	2a	3086	1/1	0.96	0.22	45,45,45,45	0
54	MG	1A	3626	1/1	0.96	0.69	30,30,30,30	0
54	MG	1a	3234	1/1	0.96	0.08	64,64,64,64	0
54	MG	2A	3153	1/1	0.96	0.29	42,42,42,42	0
54	MG	1A	3509	1/1	0.96	0.10	26,26,26,26	0
54	MG	1A	3895	1/1	0.96	0.18	17,17,17,17	0
54	MG	2A	3656	1/1	0.96	0.10	45,45,45,45	0
54	MG	2A	3396	1/1	0.96	0.15	37,37,37,37	0
54	MG	1A	3629	1/1	0.96	0.48	34,34,34,34	0
54	MG	1A	3211	1/1	0.96	0.11	27,27,27,27	0
54	MG	2A	3661	1/1	0.96	0.12	28,28,28,28	0
54	MG	1B	211	1/1	0.96	0.18	27,27,27,27	0
54	MG	1B	212	1/1	0.96	0.16	30,30,30,30	0
54	MG	1a	3046	1/1	0.96	0.17	41,41,41,41	0
54	MG	1A	3268	1/1	0.96	0.61	24,24,24,24	0
54	MG	1A	3212	1/1	0.96	0.22	41,41,41,41	0
54	MG	1A	3134	1/1	0.96	0.39	26,26,26,26	0
54	MG	1a	3246	1/1	0.96	0.10	47,47,47,47	0
54	MG	1A	3172	1/1	0.96	0.74	25,25,25,25	0
54	MG	2a	3106	1/1	0.96	0.15	46,46,46,46	0
54	MG	1a	3248	1/1	0.96	0.14	69,69,69,69	0
54	MG	1A	3908	1/1	0.96	0.09	37,37,37,37	0
54	MG	2A	3414	1/1	0.96	0.09	26,26,26,26	0
54	MG	2A	3674	1/1	0.96	0.15	42,42,42,42	0
54	MG	1a	3055	1/1	0.96	0.18	41,41,41,41	0
54	MG	1A	3912	1/1	0.96	0.16	35,35,35,35	0
54	MG	1A	3913	1/1	0.96	0.14	29,29,29,29	0
54	MG	1A	3274	1/1	0.96	0.40	51,51,51,51	0
54	MG	1A	3174	1/1	0.96	0.12	35,35,35,35	0
54	MG	1A	3424	1/1	0.96	0.17	45,45,45,45	0
54	MG	1A	3523	1/1	0.96	0.18	22,22,22,22	0
54	MG	1A	3918	1/1	0.96	0.09	37,37,37,37	0
54	MG	2A	3182	1/1	0.96	0.12	39,39,39,39	0
54	MG	2A	3425	1/1	0.96	0.52	45,45,45,45	0
54	MG	1a	3063	1/1	0.96	0.14	53,53,53,53	0
54	MG	1A	3425	1/1	0.96	0.19	21,21,21,21	0
54	MG	1A	3764	1/1	0.96	0.09	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3426	1/1	0.96	0.21	35,35,35,35	0
54	MG	1A	3643	1/1	0.96	0.12	40,40,40,40	0
54	MG	1A	3340	1/1	0.96	0.13	29,29,29,29	0
54	MG	2A	3434	1/1	0.96	0.27	55,55,55,55	0
54	MG	1A	3769	1/1	0.96	0.18	46,46,46,46	0
54	MG	1A	3036	1/1	0.96	0.12	44,44,44,44	0
54	MG	2a	3134	1/1	0.96	0.17	64,64,64,64	0
54	MG	1a	3071	1/1	0.96	0.14	62,62,62,62	0
54	MG	1A	3136	1/1	0.96	0.12	40,40,40,40	0
54	MG	1a	3073	1/1	0.96	0.12	52,52,52,52	0
54	MG	2a	3139	1/1	0.96	0.18	60,60,60,60	0
54	MG	1A	3219	1/1	0.96	0.37	43,43,43,43	0
54	MG	1a	3275	1/1	0.96	0.06	44,44,44,44	0
54	MG	2A	3700	1/1	0.96	0.22	56,56,56,56	0
54	MG	2A	3443	1/1	0.96	0.09	47,47,47,47	0
54	MG	1A	3649	1/1	0.96	0.28	57,57,57,57	0
54	MG	1A	3344	1/1	0.96	0.14	37,37,37,37	0
54	MG	1A	3775	1/1	0.96	0.14	23,23,23,23	0
54	MG	2A	3706	1/1	0.96	0.09	36,36,36,36	0
54	MG	2A	3447	1/1	0.96	0.27	49,49,49,49	0
54	MG	1a	3079	1/1	0.96	0.10	36,36,36,36	0
54	MG	1a	3080	1/1	0.96	0.16	37,37,37,37	0
54	MG	1A	3081	1/1	0.96	0.49	34,34,34,34	0
54	MG	1A	3281	1/1	0.96	0.39	22,22,22,22	0
54	MG	1A	3010	1/1	0.96	0.16	39,39,39,39	0
54	MG	2A	3207	1/1	0.96	0.14	42,42,42,42	0
54	MG	1A	3537	1/1	0.96	0.17	23,23,23,23	0
54	MG	1A	3107	1/1	0.96	0.21	26,26,26,26	0
54	MG	1e	201	1/1	0.96	0.15	44,44,44,44	0
54	MG	2a	3162	1/1	0.96	0.21	58,58,58,58	0
54	MG	2A	3719	1/1	0.96	0.18	61,61,61,61	0
54	MG	2A	3720	1/1	0.96	0.09	54,54,54,54	0
54	MG	1E	305	1/1	0.96	0.13	45,45,45,45	0
54	MG	1A	3351	1/1	0.96	0.16	9,9,9,9	0
54	MG	1A	3659	1/1	0.96	0.10	49,49,49,49	0
54	MG	1A	3353	1/1	0.96	0.14	27,27,27,27	0
54	MG	1A	3144	1/1	0.96	0.15	20,20,20,20	0
54	MG	1A	3084	1/1	0.96	0.41	34,34,34,34	0
54	MG	1F	309	1/1	0.96	0.27	29,29,29,29	0
54	MG	1A	3444	1/1	0.96	0.18	13,13,13,13	0
54	MG	1A	3550	1/1	0.96	0.12	24,24,24,24	0
54	MG	1A	3356	1/1	0.96	0.12	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3793	1/1	0.96	0.10	39,39,39,39	0
54	MG	2a	3177	1/1	0.96	0.05	69,69,69,69	0
54	MG	1A	3553	1/1	0.96	0.08	39,39,39,39	0
54	MG	1n	103	1/1	0.96	0.21	54,54,54,54	0
54	MG	1a	3100	1/1	0.96	0.18	54,54,54,54	0
54	MG	1A	3446	1/1	0.96	0.31	32,32,32,32	0
54	MG	1A	3015	1/1	0.96	0.23	37,37,37,37	0
54	MG	2A	3738	1/1	0.96	0.10	51,51,51,51	0
54	MG	1A	3797	1/1	0.96	0.08	45,45,45,45	0
54	MG	1A	3671	1/1	0.96	0.38	47,47,47,47	0
54	MG	1G	204	1/1	0.96	0.16	37,37,37,37	0
54	MG	2a	3187	1/1	0.96	0.25	62,62,62,62	0
54	MG	1A	3672	1/1	0.96	0.15	42,42,42,42	0
54	MG	1A	3957	1/1	0.96	0.09	39,39,39,39	0
54	MG	1A	3800	1/1	0.96	0.13	25,25,25,25	0
54	MG	1A	3001	1/1	0.96	0.09	26,26,26,26	0
54	MG	1A	3557	1/1	0.96	0.21	48,48,48,48	0
54	MG	2A	3238	1/1	0.96	0.56	35,35,35,35	0
54	MG	1A	3449	1/1	0.96	0.12	46,46,46,46	0
54	MG	2A	3490	1/1	0.96	0.20	62,62,62,62	0
54	MG	1A	3559	1/1	0.96	0.08	29,29,29,29	0
54	MG	2a	3198	1/1	0.96	0.21	72,72,72,72	0
54	MG	1A	3231	1/1	0.96	0.45	24,24,24,24	0
54	MG	1P	202	1/1	0.96	0.45	24,24,24,24	0
54	MG	2A	3754	1/1	0.96	0.22	47,47,47,47	0
54	MG	1A	3111	1/1	0.96	0.24	21,21,21,21	0
54	MG	1A	3565	1/1	0.96	0.08	29,29,29,29	0
54	MG	2A	3015	1/1	0.96	0.48	36,36,36,36	0
54	MG	1A	3066	1/1	0.96	0.17	20,20,20,20	0
55	YXM	1A	4055	40/40	0.96	0.34	16,31,46,48	0
55	YXM	2A	3758	40/40	0.96	0.44	28,39,51,52	0
54	MG	1A	3567	1/1	0.96	0.10	36,36,36,36	0
54	MG	2A	3499	1/1	0.96	0.14	25,25,25,25	0
54	MG	1A	3568	1/1	0.96	0.22	42,42,42,42	0
54	MG	1A	3683	1/1	0.96	0.21	45,45,45,45	0
54	MG	2A	3022	1/1	0.96	0.12	31,31,31,31	0
54	MG	1a	3128	1/1	0.96	0.08	54,54,54,54	0
54	MG	2A	3506	1/1	0.96	0.06	38,38,38,38	0
54	MG	1A	3364	1/1	0.96	0.12	45,45,45,45	0
54	MG	1A	3366	1/1	0.96	0.13	22,22,22,22	0
54	MG	1A	3296	1/1	0.96	0.24	27,27,27,27	0
54	MG	1A	3463	1/1	0.96	0.18	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3297	1/1	0.96	0.12	40,40,40,40	0
54	MG	1a	3173	1/1	0.97	0.13	54,54,54,54	0
54	MG	1A	3757	1/1	0.97	0.17	24,24,24,24	0
54	MG	2W	201	1/1	0.97	0.54	41,41,41,41	0
54	MG	1a	3024	1/1	0.97	0.15	55,55,55,55	0
54	MG	1A	3395	1/1	0.97	0.10	34,34,34,34	0
54	MG	1A	3085	1/1	0.97	0.61	37,37,37,37	0
54	MG	1A	3398	1/1	0.97	0.14	32,32,32,32	0
54	MG	1A	3213	1/1	0.97	0.62	32,32,32,32	0
54	MG	1A	3400	1/1	0.97	0.20	27,27,27,27	0
54	MG	1A	3858	1/1	0.97	0.11	48,48,48,48	0
54	MG	1A	3309	1/1	0.97	0.67	31,31,31,31	0
54	MG	1A	3860	1/1	0.97	0.16	34,34,34,34	0
54	MG	25	101	1/1	0.97	0.85	36,36,36,36	0
54	MG	2A	3609	1/1	0.97	0.11	52,52,52,52	0
54	MG	1A	3765	1/1	0.97	0.16	30,30,30,30	0
54	MG	2A	3399	1/1	0.97	0.14	50,50,50,50	0
54	MG	1E	301	1/1	0.97	0.98	42,42,42,42	0
54	MG	2A	3034	1/1	0.97	0.94	53,53,53,53	0
54	MG	2a	3002	1/1	0.97	0.30	54,54,54,54	0
54	MG	1E	302	1/1	0.97	0.25	28,28,28,28	0
54	MG	2A	3404	1/1	0.97	0.14	29,29,29,29	0
54	MG	1A	3347	1/1	0.97	0.25	33,33,33,33	0
54	MG	1A	3979	1/1	0.97	0.20	51,51,51,51	0
54	MG	1A	3980	1/1	0.97	0.06	34,34,34,34	0
54	MG	2A	3408	1/1	0.97	0.17	41,41,41,41	0
54	MG	1A	3462	1/1	0.97	0.09	45,45,45,45	0
54	MG	1F	301	1/1	0.97	0.27	20,20,20,20	0
54	MG	1A	3348	1/1	0.97	0.15	14,14,14,14	0
54	MG	1A	3310	1/1	0.97	0.32	45,45,45,45	0
54	MG	1F	304	1/1	0.97	0.29	26,26,26,26	0
54	MG	2A	3626	1/1	0.97	0.13	30,30,30,30	0
54	MG	1A	3271	1/1	0.97	0.12	36,36,36,36	0
54	MG	2A	3628	1/1	0.97	0.11	58,58,58,58	0
54	MG	1F	307	1/1	0.97	0.14	25,25,25,25	0
54	MG	1A	3466	1/1	0.97	0.14	37,37,37,37	0
54	MG	1A	3272	1/1	0.97	0.41	27,27,27,27	0
54	MG	1A	3047	1/1	0.97	0.23	36,36,36,36	0
54	MG	1A	3989	1/1	0.97	0.15	32,32,32,32	0
54	MG	1a	3054	1/1	0.97	0.15	32,32,32,32	0
54	MG	2A	3053	1/1	0.97	0.12	42,42,42,42	0
54	MG	2A	3229	1/1	0.97	0.27	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3054	1/1	0.97	0.11	37,37,37,37	0
54	MG	2A	3427	1/1	0.97	0.16	40,40,40,40	0
54	MG	2A	3640	1/1	0.97	0.11	49,49,49,49	0
54	MG	2A	3231	1/1	0.97	0.15	44,44,44,44	0
54	MG	2a	3030	1/1	0.97	0.09	53,53,53,53	0
54	MG	1A	3040	1/1	0.97	0.19	24,24,24,24	0
54	MG	1A	3610	1/1	0.97	0.21	34,34,34,34	0
54	MG	2A	3644	1/1	0.97	0.37	57,57,57,57	0
54	MG	1A	3876	1/1	0.97	0.10	38,38,38,38	0
54	MG	1A	3113	1/1	0.97	0.55	37,37,37,37	0
54	MG	1A	3994	1/1	0.97	0.13	15,15,15,15	0
54	MG	1A	3778	1/1	0.97	0.20	28,28,28,28	0
54	MG	1A	3779	1/1	0.97	0.15	38,38,38,38	0
54	MG	2A	3651	1/1	0.97	0.12	72,72,72,72	0
54	MG	1A	3173	1/1	0.97	0.45	29,29,29,29	0
54	MG	1A	3244	1/1	0.97	0.63	32,32,32,32	0
54	MG	1A	3538	1/1	0.97	0.15	24,24,24,24	0
54	MG	2A	3439	1/1	0.97	0.22	38,38,38,38	0
54	MG	1A	3783	1/1	0.97	0.09	51,51,51,51	0
54	MG	1A	3131	1/1	0.97	0.13	48,48,48,48	0
54	MG	1A	3885	1/1	0.97	0.09	30,30,30,30	0
54	MG	1A	3114	1/1	0.97	0.39	28,28,28,28	0
54	MG	2a	3049	1/1	0.97	0.19	44,44,44,44	0
54	MG	2A	3660	1/1	0.97	0.14	24,24,24,24	0
54	MG	1A	3198	1/1	0.97	0.32	50,50,50,50	0
54	MG	1A	3543	1/1	0.97	0.12	20,20,20,20	0
54	MG	1A	3544	1/1	0.97	0.93	27,27,27,27	0
54	MG	2A	3073	1/1	0.97	0.54	33,33,33,33	0
54	MG	1A	3699	1/1	0.97	0.24	16,16,16,16	0
54	MG	1A	3700	1/1	0.97	0.12	46,46,46,46	0
54	MG	1A	3115	1/1	0.97	0.39	24,24,24,24	0
54	MG	2A	3077	1/1	0.97	0.06	51,51,51,51	0
54	MG	2a	3059	1/1	0.97	0.12	53,53,53,53	0
54	MG	2A	3078	1/1	0.97	0.29	30,30,30,30	0
54	MG	1A	3546	1/1	0.97	0.15	48,48,48,48	0
54	MG	1Q	202	1/1	0.97	0.12	29,29,29,29	0
54	MG	2A	3455	1/1	0.97	0.10	51,51,51,51	0
54	MG	2A	3673	1/1	0.97	0.14	38,38,38,38	0
54	MG	1a	3077	1/1	0.97	0.13	39,39,39,39	0
54	MG	1A	3049	1/1	0.97	0.39	28,28,28,28	0
54	MG	2A	3261	1/1	0.97	0.18	58,58,58,58	0
54	MG	1Q	204	1/1	0.97	0.27	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3479	1/1	0.97	0.10	36,36,36,36	0
54	MG	1A	3365	1/1	0.97	0.22	40,40,40,40	0
54	MG	1A	3627	1/1	0.97	0.42	18,18,18,18	0
54	MG	1A	4017	1/1	0.97	0.09	60,60,60,60	0
54	MG	1R	205	1/1	0.97	0.12	20,20,20,20	0
54	MG	1A	3118	1/1	0.97	0.14	13,13,13,13	0
54	MG	2A	3270	1/1	0.97	1.05	50,50,50,50	0
54	MG	2A	3469	1/1	0.97	0.08	43,43,43,43	0
54	MG	1A	3900	1/1	0.97	0.11	28,28,28,28	0
54	MG	2a	3079	1/1	0.97	0.07	50,50,50,50	0
54	MG	2a	3080	1/1	0.97	0.12	49,49,49,49	0
54	MG	1A	3552	1/1	0.97	0.16	35,35,35,35	0
54	MG	2A	3273	1/1	0.97	0.67	48,48,48,48	0
54	MG	1A	3482	1/1	0.97	0.17	51,51,51,51	0
54	MG	1T	203	1/1	0.97	0.06	55,55,55,55	0
54	MG	1A	3904	1/1	0.97	0.24	49,49,49,49	0
54	MG	1A	3905	1/1	0.97	0.14	41,41,41,41	0
54	MG	2A	3478	1/1	0.97	0.28	52,52,52,52	0
54	MG	2A	3278	1/1	0.97	0.12	44,44,44,44	0
54	MG	1U	201	1/1	0.97	0.53	26,26,26,26	0
54	MG	1U	202	1/1	0.97	0.18	32,32,32,32	0
54	MG	1A	3907	1/1	0.97	0.23	18,18,18,18	0
54	MG	1A	3100	1/1	0.97	0.50	34,34,34,34	0
54	MG	2A	3699	1/1	0.97	0.09	44,44,44,44	0
54	MG	2A	3283	1/1	0.97	0.25	34,34,34,34	0
54	MG	1A	3028	1/1	0.97	0.27	20,20,20,20	0
54	MG	2A	3102	1/1	0.97	0.08	27,27,27,27	0
54	MG	1A	3327	1/1	0.97	0.14	42,42,42,42	0
54	MG	1A	3254	1/1	0.97	0.20	49,49,49,49	0
54	MG	1A	4030	1/1	0.97	0.15	36,36,36,36	0
54	MG	1a	3102	1/1	0.97	0.11	66,66,66,66	0
54	MG	1V	202	1/1	0.97	0.17	43,43,43,43	0
54	MG	1A	3488	1/1	0.97	0.14	47,47,47,47	0
54	MG	2A	3109	1/1	0.97	0.14	23,23,23,23	0
54	MG	1a	3105	1/1	0.97	0.21	46,46,46,46	0
54	MG	1A	3637	1/1	0.97	0.15	17,17,17,17	0
54	MG	2A	3113	1/1	0.97	0.13	42,42,42,42	0
54	MG	1a	3256	1/1	0.97	0.09	39,39,39,39	0
54	MG	2A	3715	1/1	0.97	0.28	43,43,43,43	0
54	MG	1A	3227	1/1	0.97	0.39	37,37,37,37	0
54	MG	2A	3717	1/1	0.97	0.15	38,38,38,38	0
54	MG	1A	3720	1/1	0.97	0.10	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1W	204	1/1	0.97	0.16	25,25,25,25	0
54	MG	2A	3119	1/1	0.97	0.17	49,49,49,49	0
54	MG	2a	3117	1/1	0.97	0.08	45,45,45,45	0
54	MG	2A	3504	1/1	0.97	0.09	26,26,26,26	0
54	MG	1A	3490	1/1	0.97	0.12	40,40,40,40	0
54	MG	1A	4036	1/1	0.97	0.11	47,47,47,47	0
54	MG	1A	3920	1/1	0.97	0.30	19,19,19,19	0
54	MG	2A	3305	1/1	0.97	0.09	53,53,53,53	0
54	MG	2a	3123	1/1	0.97	0.16	63,63,63,63	0
54	MG	1a	3115	1/1	0.97	0.11	44,44,44,44	0
54	MG	1a	3265	1/1	0.97	0.10	45,45,45,45	0
54	MG	2A	3125	1/1	0.97	0.15	34,34,34,34	0
54	MG	2A	3126	1/1	0.97	0.07	40,40,40,40	0
54	MG	1A	3921	1/1	0.97	0.21	16,16,16,16	0
54	MG	1A	3561	1/1	0.97	0.13	27,27,27,27	0
54	MG	1A	3427	1/1	0.97	0.18	50,50,50,50	0
54	MG	2a	3131	1/1	0.97	0.18	67,67,67,67	0
54	MG	1a	3269	1/1	0.97	0.09	70,70,70,70	0
54	MG	2A	3316	1/1	0.97	0.15	19,19,19,19	0
54	MG	1A	3564	1/1	0.97	0.12	20,20,20,20	0
54	MG	1A	3256	1/1	0.97	0.34	19,19,19,19	0
54	MG	2a	3136	1/1	0.97	0.09	47,47,47,47	0
54	MG	1A	4043	1/1	0.97	0.31	43,43,43,43	0
54	MG	1A	3294	1/1	0.97	0.18	44,44,44,44	0
54	MG	1A	3431	1/1	0.97	0.12	23,23,23,23	0
54	MG	2A	3138	1/1	0.97	0.06	59,59,59,59	0
54	MG	2a	3141	1/1	0.97	0.19	47,47,47,47	0
54	MG	2A	3742	1/1	0.97	0.14	59,59,59,59	0
54	MG	2A	3139	1/1	0.97	0.07	45,45,45,45	0
54	MG	2A	3324	1/1	0.97	0.19	38,38,38,38	0
54	MG	1A	3257	1/1	0.97	0.28	37,37,37,37	0
54	MG	1a	3126	1/1	0.97	0.07	50,50,50,50	0
54	MG	1A	3228	1/1	0.97	0.34	28,28,28,28	0
54	MG	1A	3818	1/1	0.97	0.14	29,29,29,29	0
54	MG	1A	3931	1/1	0.97	0.14	12,12,12,12	0
54	MG	1A	3819	1/1	0.97	0.23	31,31,31,31	0
54	MG	1A	3261	1/1	0.97	0.14	33,33,33,33	0
54	MG	2A	3534	1/1	0.97	0.11	50,50,50,50	0
54	MG	1A	3379	1/1	0.97	0.17	33,33,33,33	0
54	MG	2a	3154	1/1	0.97	0.11	50,50,50,50	0
54	MG	1A	3091	1/1	0.97	0.53	34,34,34,34	0
54	MG	1A	3381	1/1	0.97	0.16	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3736	1/1	0.97	0.08	15,15,15,15	0
54	MG	1A	3299	1/1	0.97	0.12	28,28,28,28	0
54	MG	1A	3829	1/1	0.97	0.23	40,40,40,40	0
54	MG	1A	3575	1/1	0.97	0.11	46,46,46,46	0
54	MG	2A	3542	1/1	0.97	0.13	42,42,42,42	0
54	MG	2B	204	1/1	0.97	0.06	76,76,76,76	0
54	MG	2A	3340	1/1	0.97	0.12	27,27,27,27	0
54	MG	15	107	1/1	0.97	0.07	63,63,63,63	0
54	MG	2a	3167	1/1	0.97	0.15	65,65,65,65	0
54	MG	2A	3545	1/1	0.97	0.05	47,47,47,47	0
54	MG	1A	3502	1/1	0.97	0.27	15,15,15,15	0
54	MG	1A	3942	1/1	0.97	0.10	52,52,52,52	0
54	MG	1A	3577	1/1	0.97	0.10	35,35,35,35	0
54	MG	2A	3158	1/1	0.97	0.09	47,47,47,47	0
54	MG	1A	3140	1/1	0.97	0.14	25,25,25,25	0
54	MG	2A	3551	1/1	0.97	0.38	30,30,30,30	0
54	MG	1A	3742	1/1	0.97	0.11	39,39,39,39	0
54	MG	2A	3161	1/1	0.97	0.12	42,42,42,42	0
54	MG	2A	3162	1/1	0.97	0.29	48,48,48,48	0
54	MG	1l	201	1/1	0.97	0.26	55,55,55,55	0
54	MG	1A	3385	1/1	0.97	0.18	40,40,40,40	0
54	MG	1A	3386	1/1	0.97	0.14	30,30,30,30	0
54	MG	1a	3148	1/1	0.97	0.08	48,48,48,48	0
54	MG	1A	3025	1/1	0.97	0.57	40,40,40,40	0
54	MG	1A	3950	1/1	0.97	0.15	48,48,48,48	0
54	MG	1A	3838	1/1	0.97	0.64	28,28,28,28	0
54	MG	1B	215	1/1	0.97	0.11	50,50,50,50	0
54	MG	1A	3388	1/1	0.97	0.09	36,36,36,36	0
54	MG	1A	3664	1/1	0.97	0.14	28,28,28,28	0
54	MG	1A	3004	1/1	0.97	0.17	30,30,30,30	0
54	MG	1A	3666	1/1	0.97	0.12	34,34,34,34	0
54	MG	2A	3568	1/1	0.97	0.09	52,52,52,52	0
54	MG	1a	3158	1/1	0.97	0.10	47,47,47,47	0
54	MG	1A	3164	1/1	0.97	0.10	23,23,23,23	0
54	MG	1A	3006	1/1	0.97	0.19	20,20,20,20	0
54	MG	2A	3180	1/1	0.97	0.28	58,58,58,58	0
54	MG	1B	222	1/1	0.97	0.22	45,45,45,45	0
54	MG	2A	3367	1/1	0.97	0.12	28,28,28,28	0
54	MG	1A	3588	1/1	0.97	0.10	35,35,35,35	0
54	MG	1A	3847	1/1	0.97	0.12	31,31,31,31	0
54	MG	1A	3961	1/1	0.97	0.15	38,38,38,38	0
54	MG	2A	3579	1/1	0.97	0.11	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3010	1/1	0.97	0.14	58,58,58,58	0
54	MG	1A	3753	1/1	0.97	0.11	27,27,27,27	0
54	MG	1B	227	1/1	0.97	0.20	65,65,65,65	0
54	MG	2A	3583	1/1	0.97	0.13	26,26,26,26	0
54	MG	2t	3100	1/1	0.97	0.12	48,48,48,48	0
54	MG	2A	3376	1/1	0.97	0.11	50,50,50,50	0
54	MG	2A	3189	1/1	0.97	0.21	62,62,62,62	0
54	MG	1A	3511	1/1	0.97	0.13	26,26,26,26	0
54	MG	2A	3379	1/1	0.97	0.13	38,38,38,38	0
56	MPD	18	102	8/8	0.97	0.39	28,33,38,41	0
54	MG	2Q	201	1/1	0.97	0.12	60,60,60,60	0
54	MG	2A	3589	1/1	0.97	0.18	51,51,51,51	0
54	MG	1A	3039	1/1	0.97	0.10	34,34,34,34	0
54	MG	1A	3965	1/1	0.97	0.14	17,17,17,17	0
54	MG	1A	3513	1/1	0.97	0.21	40,40,40,40	0
54	MG	2A	3017	1/1	0.97	0.47	45,45,45,45	0
54	MG	1A	3967	1/1	0.97	0.18	14,14,14,14	0
54	MG	2A	3595	1/1	0.97	0.11	50,50,50,50	0
54	MG	2A	3196	1/1	0.97	0.12	47,47,47,47	0
54	MG	2A	3019	1/1	0.97	0.38	54,54,54,54	0
54	MG	1a	3114	1/1	0.98	0.10	28,28,28,28	0
54	MG	2A	3588	1/1	0.98	0.06	40,40,40,40	0
54	MG	2A	3041	1/1	0.98	0.14	39,39,39,39	0
54	MG	1A	3357	1/1	0.98	0.15	31,31,31,31	0
54	MG	1A	3525	1/1	0.98	0.20	51,51,51,51	0
54	MG	1A	3169	1/1	0.98	0.14	36,36,36,36	0
54	MG	1A	3192	1/1	0.98	0.12	44,44,44,44	0
54	MG	1A	4014	1/1	0.98	0.15	41,41,41,41	0
54	MG	1A	3280	1/1	0.98	0.14	15,15,15,15	0
54	MG	2A	3175	1/1	0.98	0.22	41,41,41,41	0
54	MG	2A	3308	1/1	0.98	0.10	27,27,27,27	0
54	MG	1A	3595	1/1	0.98	0.19	18,18,18,18	0
54	MG	2A	3177	1/1	0.98	0.20	33,33,33,33	0
54	MG	1a	3236	1/1	0.98	0.13	52,52,52,52	0
54	MG	1A	3596	1/1	0.98	0.19	35,35,35,35	0
54	MG	1A	3597	1/1	0.98	0.30	43,43,43,43	0
54	MG	2A	3314	1/1	0.98	0.11	47,47,47,47	0
54	MG	1A	3170	1/1	0.98	0.18	29,29,29,29	0
54	MG	2a	3078	1/1	0.98	0.15	33,33,33,33	0
54	MG	1A	3362	1/1	0.98	0.22	45,45,45,45	0
54	MG	1A	3282	1/1	0.98	0.29	18,18,18,18	0
54	MG	2A	3184	1/1	0.98	0.32	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1a	3018	1/1	0.98	0.18	35,35,35,35	0
54	MG	2A	3057	1/1	0.98	0.07	53,53,53,53	0
54	MG	2a	3084	1/1	0.98	0.14	50,50,50,50	0
54	MG	2A	3461	1/1	0.98	0.10	44,44,44,44	0
54	MG	1A	3283	1/1	0.98	0.41	40,40,40,40	0
54	MG	1A	3194	1/1	0.98	0.18	49,49,49,49	0
54	MG	1a	3021	1/1	0.98	0.07	36,36,36,36	0
54	MG	1A	3250	1/1	0.98	0.32	32,32,32,32	0
54	MG	2A	3466	1/1	0.98	0.30	58,58,58,58	0
54	MG	1A	3367	1/1	0.98	0.11	28,28,28,28	0
54	MG	2a	3092	1/1	0.98	0.11	53,53,53,53	0
54	MG	1A	4026	1/1	0.98	0.22	10,10,10,10	0
54	MG	1A	3536	1/1	0.98	0.06	43,43,43,43	0
54	MG	1A	3842	1/1	0.98	0.10	24,24,24,24	0
54	MG	1a	3251	1/1	0.98	0.12	39,39,39,39	0
54	MG	1A	3195	1/1	0.98	0.46	36,36,36,36	0
54	MG	2A	3473	1/1	0.98	0.16	42,42,42,42	0
54	MG	1A	3418	1/1	0.98	0.13	14,14,14,14	0
54	MG	2A	3624	1/1	0.98	0.10	32,32,32,32	0
54	MG	1A	3126	1/1	0.98	0.19	23,23,23,23	0
54	MG	2D	302	1/1	0.98	1.25	42,42,42,42	0
54	MG	1a	3140	1/1	0.98	0.06	49,49,49,49	0
54	MG	1A	3540	1/1	0.98	0.18	16,16,16,16	0
54	MG	1A	3017	1/1	0.98	0.38	17,17,17,17	0
54	MG	1A	3685	1/1	0.98	0.15	40,40,40,40	0
54	MG	1A	3076	1/1	0.98	0.35	23,23,23,23	0
54	MG	2A	3338	1/1	0.98	0.13	24,24,24,24	0
54	MG	2A	3632	1/1	0.98	0.09	40,40,40,40	0
54	MG	1A	3422	1/1	0.98	0.11	31,31,31,31	0
54	MG	1A	3225	1/1	0.98	0.39	28,28,28,28	0
54	MG	1a	3036	1/1	0.98	0.12	50,50,50,50	0
54	MG	1A	3292	1/1	0.98	0.14	14,14,14,14	0
54	MG	1A	3483	1/1	0.98	0.10	35,35,35,35	0
54	MG	1A	3042	1/1	0.98	0.15	24,24,24,24	0
54	MG	1A	3013	1/1	0.98	0.25	21,21,21,21	0
54	MG	2E	305	1/1	0.98	0.12	23,23,23,23	0
54	MG	2A	3489	1/1	0.98	0.09	29,29,29,29	0
54	MG	1a	3152	1/1	0.98	0.14	47,47,47,47	0
54	MG	1A	3079	1/1	0.98	0.31	29,29,29,29	0
54	MG	1A	3948	1/1	0.98	0.11	27,27,27,27	0
54	MG	1A	3428	1/1	0.98	0.14	22,22,22,22	0
54	MG	2A	3086	1/1	0.98	0.12	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3334	1/1	0.98	0.06	55,55,55,55	0
54	MG	1a	3045	1/1	0.98	0.16	41,41,41,41	0
54	MG	1A	3776	1/1	0.98	0.08	30,30,30,30	0
54	MG	1A	3378	1/1	0.98	0.15	13,13,13,13	0
54	MG	1a	3048	1/1	0.98	0.17	40,40,40,40	0
54	MG	1A	3259	1/1	0.98	0.15	65,65,65,65	0
54	MG	1A	3260	1/1	0.98	0.11	39,39,39,39	0
54	MG	1A	3625	1/1	0.98	0.57	28,28,28,28	0
54	MG	1A	3080	1/1	0.98	0.41	29,29,29,29	0
54	MG	1T	204	1/1	0.98	0.11	48,48,48,48	0
54	MG	1a	3166	1/1	0.98	0.20	65,65,65,65	0
54	MG	1A	3865	1/1	0.98	0.41	31,31,31,31	0
54	MG	1A	3230	1/1	0.98	0.43	32,32,32,32	0
54	MG	1A	3068	1/1	0.98	0.25	30,30,30,30	0
54	MG	1A	3960	1/1	0.98	0.28	40,40,40,40	0
54	MG	1A	3868	1/1	0.98	0.16	40,40,40,40	0
54	MG	1A	3869	1/1	0.98	0.14	53,53,53,53	0
54	MG	1U	205	1/1	0.98	0.24	24,24,24,24	0
54	MG	2A	3234	1/1	0.98	0.82	45,45,45,45	0
54	MG	1g	201	1/1	0.98	0.23	50,50,50,50	0
54	MG	2W	202	1/1	0.98	0.20	53,53,53,53	0
54	MG	2A	3371	1/1	0.98	0.10	25,25,25,25	0
54	MG	1A	3204	1/1	0.98	0.44	30,30,30,30	0
54	MG	1A	3437	1/1	0.98	0.08	48,48,48,48	0
54	MG	1A	3302	1/1	0.98	0.32	20,20,20,20	0
54	MG	2A	3375	1/1	0.98	0.07	40,40,40,40	0
54	MG	1h	202	1/1	0.98	0.17	61,61,61,61	0
54	MG	2A	3110	1/1	0.98	0.21	50,50,50,50	0
54	MG	1A	3233	1/1	0.98	0.31	28,28,28,28	0
54	MG	1A	3874	1/1	0.98	0.12	34,34,34,34	0
54	MG	1A	3707	1/1	0.98	0.15	26,26,26,26	0
54	MG	1A	3563	1/1	0.98	0.18	25,25,25,25	0
54	MG	2a	3157	1/1	0.98	0.15	41,41,41,41	0
54	MG	1A	3003	1/1	0.98	0.12	24,24,24,24	0
54	MG	1A	3635	1/1	0.98	0.06	41,41,41,41	0
54	MG	2a	3160	1/1	0.98	0.09	57,57,57,57	0
54	MG	2A	3117	1/1	0.98	0.18	39,39,39,39	0
54	MG	1A	3083	1/1	0.98	0.40	25,25,25,25	0
54	MG	1A	3390	1/1	0.98	0.11	28,28,28,28	0
54	MG	1A	3029	1/1	0.98	0.32	38,38,38,38	0
54	MG	1A	3392	1/1	0.98	0.06	56,56,56,56	0
54	MG	2A	3252	1/1	0.98	0.32	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3030	1/1	0.98	0.13	24,24,24,24	0
54	MG	1A	3101	1/1	0.98	0.36	30,30,30,30	0
54	MG	1A	3718	1/1	0.98	0.13	41,41,41,41	0
54	MG	1A	3139	1/1	0.98	0.13	21,21,21,21	0
54	MG	1A	3072	1/1	0.98	0.21	24,24,24,24	0
54	MG	1A	3644	1/1	0.98	0.15	18,18,18,18	0
54	MG	1A	3141	1/1	0.98	0.25	28,28,28,28	0
54	MG	1A	3450	1/1	0.98	0.15	30,30,30,30	0
54	MG	2A	3004	1/1	0.98	0.13	28,28,28,28	0
54	MG	1A	3103	1/1	0.98	0.25	20,20,20,20	0
54	MG	1a	3084	1/1	0.98	0.28	70,70,70,70	0
54	MG	2A	3007	1/1	0.98	0.19	37,37,37,37	0
54	MG	2a	3018	1/1	0.98	0.12	40,40,40,40	0
54	MG	2A	3008	1/1	0.98	0.28	35,35,35,35	0
54	MG	2A	3403	1/1	0.98	0.10	28,28,28,28	0
54	MG	1A	3352	1/1	0.98	0.14	31,31,31,31	0
54	MG	2A	3701	1/1	0.98	0.11	30,30,30,30	0
54	MG	2A	3137	1/1	0.98	0.19	21,21,21,21	0
54	MG	1A	3986	1/1	0.98	0.13	24,24,24,24	0
54	MG	1A	3893	1/1	0.98	0.14	24,24,24,24	0
54	MG	1A	3401	1/1	0.98	0.16	25,25,25,25	0
54	MG	1A	3727	1/1	0.98	0.37	33,33,33,33	0
54	MG	1D	304	1/1	0.98	0.15	19,19,19,19	0
54	MG	2a	3190	1/1	0.98	0.12	60,60,60,60	0
54	MG	1A	3578	1/1	0.98	0.12	31,31,31,31	0
54	MG	2A	3412	1/1	0.98	0.12	27,27,27,27	0
54	MG	1A	3024	1/1	0.98	0.15	12,12,12,12	0
54	MG	1a	3206	1/1	0.98	0.13	64,64,64,64	0
54	MG	2A	3561	1/1	0.98	0.20	43,43,43,43	0
54	MG	1A	3810	1/1	0.98	0.09	56,56,56,56	0
54	MG	1A	3456	1/1	0.98	0.10	43,43,43,43	0
54	MG	1A	3653	1/1	0.98	0.27	42,42,42,42	0
54	MG	2A	3418	1/1	0.98	0.07	28,28,28,28	0
54	MG	1A	3901	1/1	0.98	0.08	24,24,24,24	0
54	MG	1A	3654	1/1	0.98	0.52	20,20,20,20	0
54	MG	1A	3457	1/1	0.98	0.13	44,44,44,44	0
54	MG	1a	3099	1/1	0.98	0.10	54,54,54,54	0
54	MG	1A	3516	1/1	0.98	0.20	25,25,25,25	0
54	MG	2A	3571	1/1	0.98	0.11	38,38,38,38	0
54	MG	2a	3044	1/1	0.98	0.09	55,55,55,55	0
54	MG	1A	3314	1/1	0.98	0.26	31,31,31,31	0
54	MG	1A	3518	1/1	0.98	0.17	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3426	1/1	0.98	0.46	57,57,57,57	0
54	MG	1A	3585	1/1	0.98	0.27	31,31,31,31	0
54	MG	2A	3288	1/1	0.98	0.07	48,48,48,48	0
54	MG	1A	3910	1/1	0.98	0.11	37,37,37,37	0
54	MG	1A	3911	1/1	0.98	0.16	22,22,22,22	0
54	MG	19	102	1/1	0.98	0.24	34,34,34,34	0
54	MG	1A	3020	1/1	0.98	0.59	33,33,33,33	0
54	MG	1a	3108	1/1	0.98	0.12	63,63,63,63	0
54	MG	1A	3460	1/1	0.98	0.14	15,15,15,15	0
58	ZN	1Y	501	1/1	0.98	0.15	62,62,62,62	0
54	MG	1A	3089	1/1	0.98	0.25	28,28,28,28	0
58	ZN	1n	104	1/1	0.98	0.11	64,64,64,64	0
54	MG	1A	3522	1/1	0.98	0.11	36,36,36,36	0
54	MG	1A	3823	1/1	0.98	0.10	37,37,37,37	0
58	ZN	25	102	1/1	0.98	0.19	53,53,53,53	0
58	ZN	26	501	1/1	0.98	0.17	58,58,58,58	0
58	ZN	29	501	1/1	0.98	0.12	64,64,64,64	0
54	MG	1A	4009	1/1	0.98	0.15	14,14,14,14	0
59	SF4	2d	501	8/8	0.98	0.15	56,69,75,79	0
54	MG	1D	311	1/1	0.99	0.34	18,18,18,18	0
54	MG	2A	3047	1/1	0.99	0.13	49,49,49,49	0
54	MG	1A	3397	1/1	0.99	0.11	34,34,34,34	0
54	MG	2a	3108	1/1	0.99	0.13	48,48,48,48	0
54	MG	1A	3710	1/1	0.99	0.17	22,22,22,22	0
54	MG	1a	3050	1/1	0.99	0.15	43,43,43,43	0
54	MG	1A	3620	1/1	0.99	0.13	36,36,36,36	0
54	MG	1a	3263	1/1	0.99	0.10	38,38,38,38	0
54	MG	1A	3112	1/1	0.99	0.08	41,41,41,41	0
54	MG	1A	3524	1/1	0.99	0.10	49,49,49,49	0
54	MG	1A	3453	1/1	0.99	0.10	39,39,39,39	0
54	MG	1A	3731	1/1	0.99	0.09	23,23,23,23	0
54	MG	1A	3382	1/1	0.99	0.21	51,51,51,51	0
54	MG	1A	3291	1/1	0.99	0.13	18,18,18,18	0
54	MG	2A	3520	1/1	0.99	0.14	46,46,46,46	0
54	MG	1A	3142	1/1	0.99	0.22	26,26,26,26	0
54	MG	1a	3177	1/1	0.99	0.07	57,57,57,57	0
54	MG	2A	3269	1/1	0.99	0.15	18,18,18,18	0
54	MG	2A	3129	1/1	0.99	0.50	31,31,31,31	0
54	MG	1A	3468	1/1	0.99	0.13	14,14,14,14	0
54	MG	1A	3160	1/1	0.99	0.27	28,28,28,28	0
54	MG	11	103	1/1	0.99	0.23	39,39,39,39	0
54	MG	1A	3906	1/1	0.99	0.23	26,26,26,26	0

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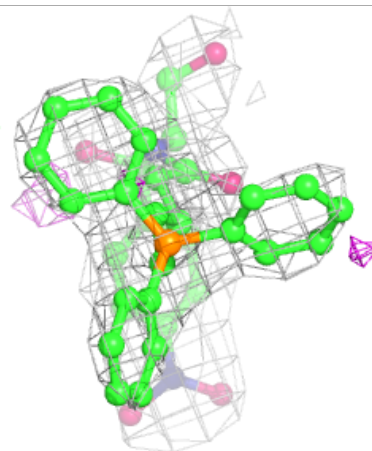
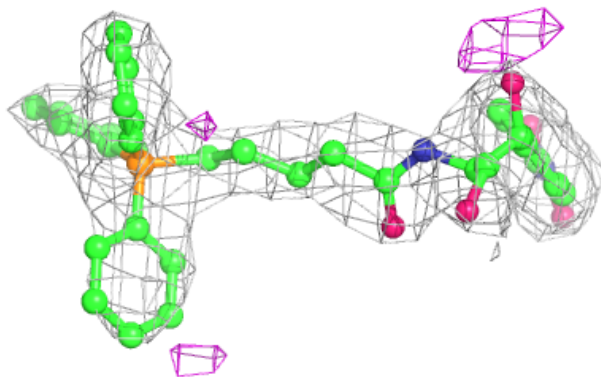
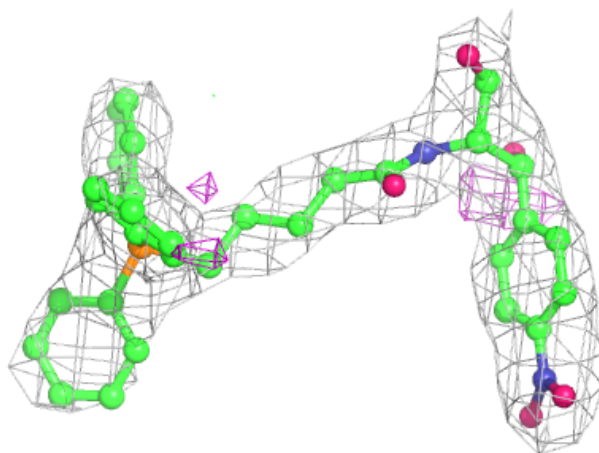
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3031	1/1	0.99	0.17	24,24,24,24	0
54	MG	1A	3032	1/1	0.99	0.12	36,36,36,36	0
54	MG	2A	3723	1/1	0.99	0.22	48,48,48,48	0
54	MG	1A	3827	1/1	0.99	0.36	27,27,27,27	0
54	MG	1A	3909	1/1	0.99	0.13	15,15,15,15	0
54	MG	1A	3828	1/1	0.99	0.09	40,40,40,40	0
54	MG	2A	3648	1/1	0.99	0.06	35,35,35,35	0
54	MG	1a	3125	1/1	0.99	0.15	24,24,24,24	0
54	MG	1F	306	1/1	0.99	0.28	24,24,24,24	0
54	MG	1A	3116	1/1	0.99	0.32	27,27,27,27	0
58	ZN	15	108	1/1	0.99	0.20	42,42,42,42	0
58	ZN	16	102	1/1	0.99	0.24	36,36,36,36	0
58	ZN	19	104	1/1	0.99	0.22	45,45,45,45	0
54	MG	1A	3157	1/1	0.99	0.44	29,29,29,29	0
54	MG	1A	3547	1/1	0.99	0.14	22,22,22,22	0
54	MG	2A	3501	1/1	0.99	0.12	52,52,52,52	0
54	MG	1A	3461	1/1	0.99	0.23	32,32,32,32	0
54	MG	1V	203	1/1	0.99	0.22	43,43,43,43	0
54	MG	1A	3759	1/1	0.99	0.21	31,31,31,31	0
54	MG	1V	205	1/1	0.99	0.12	67,67,67,67	0
59	SF4	1d	306	8/8	0.99	0.15	47,53,61,66	0
54	MG	1Q	205	1/1	0.99	0.18	27,27,27,27	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.

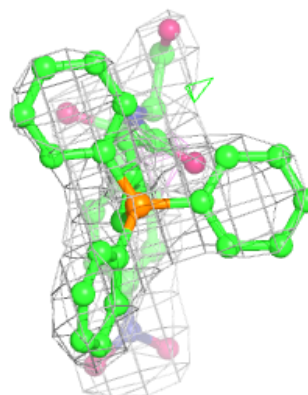
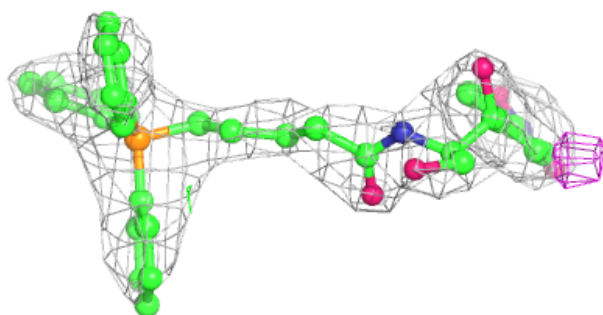
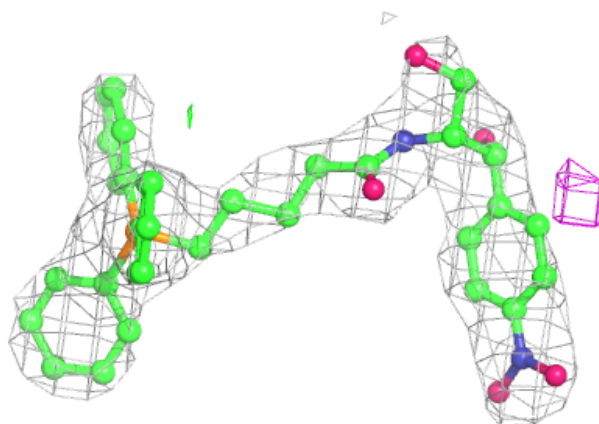
Electron density around YXM 1A 4055:

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



Electron density around YXM 2A 3758:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.