



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 5, 2021 – 09:32 PM EDT

PDB ID : 7RQ8
Title : Crystal structure of the wild-type *Thermus thermophilus* 70S ribosome in complex with iboxamycin, mRNA, deacylated A- and E-site tRNAs, and aminoacylated P-site tRNA at 2.50Å resolution
Authors : Mitcheltree, M.J.; Pisipati, A.; Syroegin, E.A.; Silvestre, K.J.; Klepacki, D.; Mason, J.D.; Terwilliger, D.W.; Testolin, G.; Pote, A.R.; Wu, K.J.Y.; Ladley, R.P.; Chatman, K.; Mankin, A.S.; Polikanov, Y.S.; Myers, A.G.
Deposited on : 2021-08-06
Resolution : 2.50 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	:	2.23.2
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)	:	2.23.2

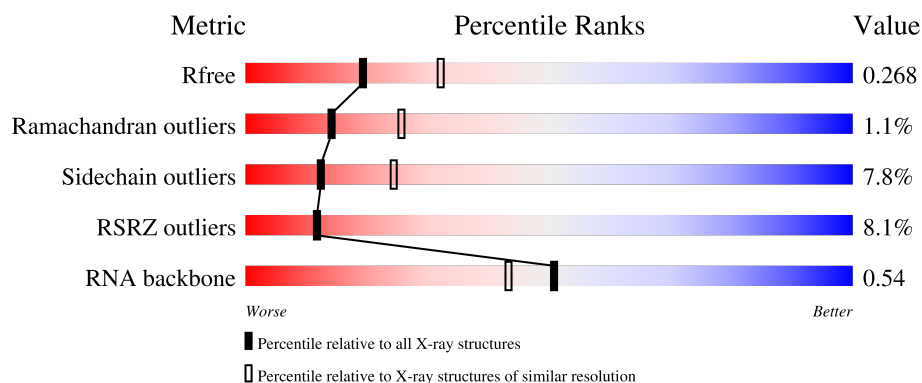
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)
RNA backbone	3102	1008 (2.84-2.16)

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>2%</div> <div> <div></div> <div>82%</div> <div>16%</div> <div>..</div> </div> </div>
1	2A	2915	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>17%</div> <div>.</div> </div> </div>
2	1B	121	<div> <div></div> <div> <div></div> <div>92%</div> <div>7%</div> <div>.</div> </div> </div>
2	2B	121	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>24%</div> <div>.</div> </div> </div>
3	1D	276	<div> <div>0%</div> <div> <div></div> <div>94%</div> <div>5%</div> <div>.</div> </div> </div>

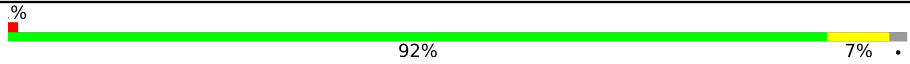
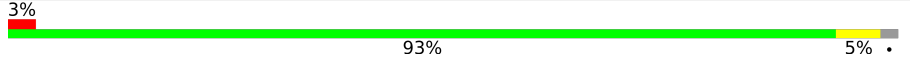
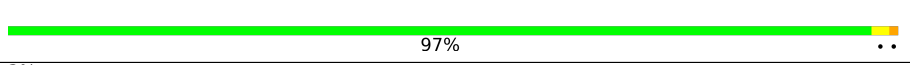
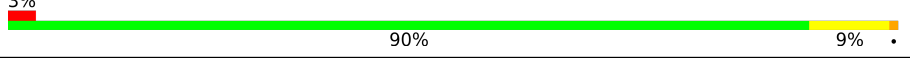
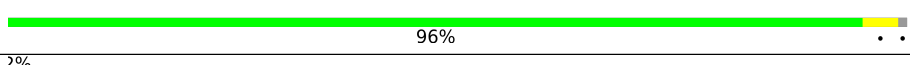
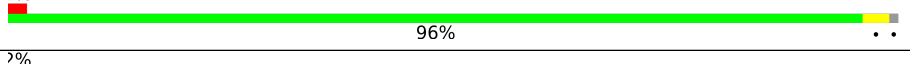
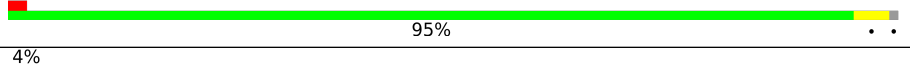
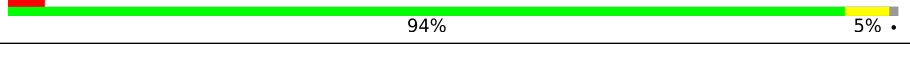
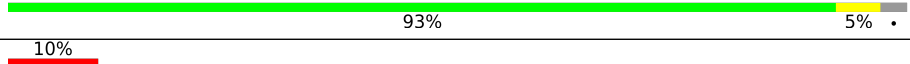


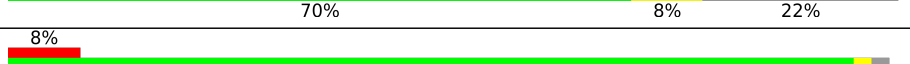
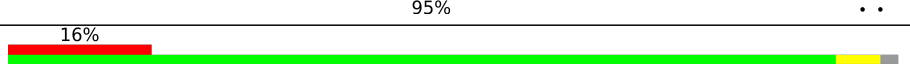
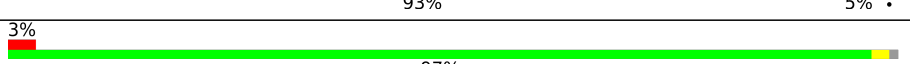
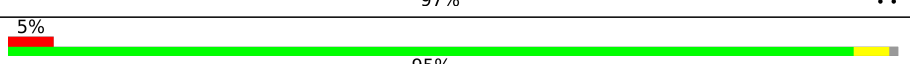
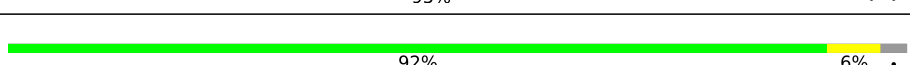

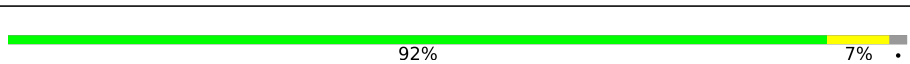
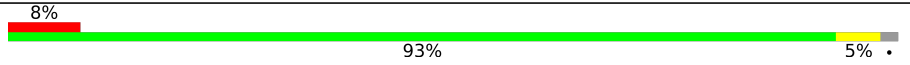


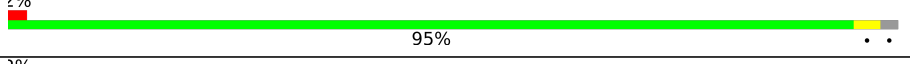
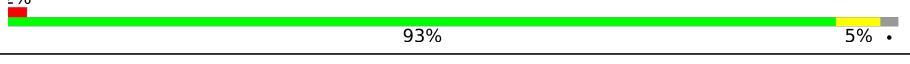


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Mol	Chain	Length	Quality of chain
3	2D	276	<div> <div>4%</div> <div>96%</div> <div>.</div> </div>
4	1E	206	<div> <div></div> <div>92%</div> <div>7% .</div> </div>
4	2E	206	<div> <div>3%</div> <div>94%</div> <div>5% .</div> </div>
5	1F	210	<div> <div></div> <div>90%</div> <div>6% .</div> </div>
5	2F	210	<div> <div>2%</div> <div>92%</div> <div>. .</div> </div>
6	1G	182	<div> <div>2%</div> <div>92%</div> <div>7% ..</div> </div>
6	2G	182	<div> <div>20%</div> <div>87%</div> <div>12% ..</div> </div>
7	1H	180	<div> <div></div> <div>93%</div> <div>. .</div> </div>
7	2H	180	<div> <div>53%</div> <div>88%</div> <div>8% .</div> </div>
8	1I	148	<div> <div>%</div> <div>86%</div> <div>12% .</div> </div>
8	2I	148	<div> <div>22%</div> <div>90%</div> <div>9% .</div> </div>
9	1N	140	<div> <div></div> <div>95%</div> <div>5%</div> </div>
9	2N	140	<div> <div>9%</div> <div>94%</div> <div>6%</div> </div>
10	1O	122	<div> <div>%</div> <div>98%</div> <div>.</div> </div>
10	2O	122	<div> <div>7%</div> <div>97%</div> <div>.</div> </div>
11	1P	150	<div> <div>%</div> <div>92%</div> <div>7% .</div> </div>
11	2P	150	<div> <div>8%</div> <div>91%</div> <div>8% .</div> </div>
12	1Q	141	<div> <div>2%</div> <div>96%</div> <div>.</div> </div>
12	2Q	141	<div> <div>23%</div> <div>95%</div> <div>5%</div> </div>
13	1R	118	<div> <div></div> <div>97%</div> <div>.</div> </div>
13	2R	118	<div> <div>3%</div> <div>97%</div> <div>.</div> </div>
14	1S	112	<div> <div>%</div> <div>91%</div> <div>7% .</div> </div>
14	2S	112	<div> <div>17%</div> <div>83%</div> <div>15% .</div> </div>
15	1T	146	<div> <div>3%</div> <div>86%</div> <div>. 10%</div> </div>
15	2T	146	<div> <div>4%</div> <div>85%</div> <div>5% 10%</div> </div>

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Mol	Chain	Length	Quality of chain
16	1U	118	
16	2U	118	
17	1V	101	
17	2V	101	
18	1W	113	
18	2W	113	
19	1X	96	
19	2X	96	
20	1Y	110	
20	2Y	110	
21	1Z	206	
21	2Z	206	
22	10	85	
22	20	85	
23	11	98	
23	21	98	
24	12	72	
24	22	72	
25	13	60	
25	23	60	
26	14	71	
26	24	71	
27	15	60	
27	25	60	
28	16	54	

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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	1v	24	

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Mol	Chain	Length	Quality of chain
53	2v	24	
54	1w	76	
54	2w	76	
55	1x	77	
55	2x	77	
56	1y	76	
56	2y	76	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	1A	3553	-	-	-	X
57	MG	1E	303	-	-	-	X
57	MG	1O	201	-	-	-	X
57	MG	1a	1758	-	-	-	X
57	MG	2A	3544	-	-	-	X
57	MG	2A	3556	-	-	-	X
57	MG	2a	1616	-	-	-	X

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 299504 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1A	2871	Total	C	N	O	P	0	0	0
			61852	27531	11572	19878	2871			
1	2A	2800	Total	C	N	O	P	0	0	0
			60322	26848	11284	19390	2800			

- Molecule 2 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1B	120	Total	C	N	O	P	0	0	0
			2577	1146	476	835	120			
2	2B	120	Total	C	N	O	P	0	0	0
			2575	1146	476	833	120			

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	1D	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			
3	2D	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	1F	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
			1423	913	253	253	4			
6	2G	181	Total	C	N	O	S	0	0	0
			1428	913	258	253	4			

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	1H	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			
7	2H	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	1I	146	Total	C	N	O	S	0	0	0
			1097	701	191	204	1			
8	2I	146	Total	C	N	O	S	0	0	0
			1064	681	186	196	1			

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	1N	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			
9	2N	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	1O	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	2O	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	1P	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			
11	2P	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	1Q	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
12	2Q	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	1R	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
13	2R	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	1S	110	Total	C	N	O	0	0	0
			873	550	174	149			
14	2S	110	Total	C	N	O	0	0	0
			870	549	173	148			

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	1T	131	Total	C	N	O	S	0	0	0
			1091	680	225	185	1			
15	2T	131	Total	C	N	O	S	0	0	0
			1083	675	224	183	1			

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	1U	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			
16	2U	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	1V	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			
17	2V	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	1W	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			
18	2W	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	1X	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			
19	2X	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	1Y	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			
20	2Y	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	1Z	154	Total	C	N	O	S	0	0	0
			1240	795	222	220	3			
21	2Z	160	Total	C	N	O	S	0	0	0
			1271	814	228	227	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	10	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			
22	20	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	11	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			
23	21	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	12	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			
24	22	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
25	13	59	Total	C	N	O	0	0	0
			469	298	90	81			
25	23	59	Total	C	N	O	0	0	0
			464	296	90	78			

- Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	14	69	Total	C	N	O	S	0	0	0
			552	349	99	99	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	24	69	Total	C	N	O	S	0	0	0
			532	339	97	91	5			

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	15	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			
27	25	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	16	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			
28	26	53	Total	C	N	O	S	0	0	0
			449	279	91	75	4			

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	17	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			
29	27	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	18	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			
30	28	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	19	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
31	29	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 32 is a RNA chain called 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	1a	1500	Total	C	N	O	P	0	0	0
			32246	14358	5975	10413	1500			
32	2a	1503	Total	C	N	O	P	0	0	0
			32327	14396	5990	10438	1503			

- Molecule 33 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	1b	231	Total	C	N	O	S	0	0	0
			1846	1179	331	331	5			
33	2b	231	Total	C	N	O	S	0	0	0
			1825	1167	326	327	5			

- Molecule 34 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	1c	206	Total	C	N	O	S	0	0	0
			1548	973	301	273	1			
34	2c	206	Total	C	N	O	S	0	0	0
			1542	968	300	273	1			

- Molecule 35 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	1d	208	Total	C	N	O	S	0	0	0
			1655	1038	326	284	7			
35	2d	208	Total	C	N	O	S	0	0	0
			1674	1050	333	284	7			

- Molecule 36 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	1e	148	Total	C	N	O	S	0	0	0
			1129	714	213	198	4			
36	2e	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			

- Molecule 37 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	1f	100	Total	C	N	O	S	0	0	0
			810	514	144	149	3			
37	2f	100	Total	C	N	O	S	0	0	0
			816	516	146	151	3			

- Molecule 38 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	1g	155	Total	C	N	O	S	0	0	0
			1231	766	243	216	6			
38	2g	155	Total	C	N	O	S	0	0	0
			1235	769	244	216	6			

- Molecule 39 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	1h	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			
39	2h	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			

- Molecule 40 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	1i	127	Total	C	N	O	0	0	0
			983	623	193	167			
40	2i	127	Total	C	N	O	0	0	0
			978	619	190	169			

- Molecule 41 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
41	1j	97	Total	C	N	O	0	0	0
			709	440	138	131			
41	2j	96	Total	C	N	O	0	0	0
			714	445	138	131			

- Molecule 42 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	1k	114	Total	C	N	O	S	0	0	0
			829	516	155	155	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	2k	114	Total	C	N	O	S	0	0	0
			833	519	156	155	3			

- Molecule 43 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	1l	122	Total	C	N	O	S	0	0	0
			932	586	185	159	2			
43	2l	122	Total	C	N	O	S	0	0	0
			932	586	185	159	2			

- Molecule 44 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	1m	123	Total	C	N	O	S	0	0	0
			958	592	198	166	2			
44	2m	122	Total	C	N	O	S	0	0	0
			950	586	197	165	2			

- Molecule 45 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	1n	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
45	2n	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 46 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	1o	88	Total	C	N	O	S	0	0	0
			728	456	144	126	2			
46	2o	88	Total	C	N	O	S	0	0	0
			728	456	144	126	2			

- Molecule 47 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	1p	82	Total	C	N	O	S	0	0	0
			681	433	134	113	1			
47	2p	82	Total	C	N	O	S	0	0	0
			677	430	133	113	1			

- Molecule 48 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	1q	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			
48	2q	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 49 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	1r	68	Total	C	N	O		0	0	0
			555	355	108	92				
49	2r	68	Total	C	N	O		0	0	0
			555	355	108	92				

- Molecule 50 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	1s	83	Total	C	N	O	S	0	0	0
			652	417	120	113	2			
50	2s	83	Total	C	N	O	S	0	0	0
			646	412	119	113	2			

- Molecule 51 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	1t	96	Total	C	N	O	S	0	0	0
			728	446	156	124	2			
51	2t	96	Total	C	N	O	S	0	0	0
			727	446	155	124	2			

- Molecule 52 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
52	1u	23	Total	C	N	O	0	0	0
			199	122	48	29			
52	2u	23	Total	C	N	O	0	0	0
			199	122	48	29			

- Molecule 53 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1v	13	Total	C	N	O	P	0	0	0
			277	125	51	88	13			
53	2v	13	Total	C	N	O	P	0	0	0
			277	125	51	88	13			

- Molecule 54 is a RNA chain called A-site tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	1w	71	Total	C	N	O	P	S	0	0
			1530	685	274	498	71	2		
54	2w	69	Total	C	N	O	P	S	0	0
			1482	662	267	482	69	2		

- Molecule 55 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	1x	76	Total	C	N	O	P	S	0	0
			1635	731	296	530	76	2		
55	2x	76	Total	C	N	O	P	S	0	0
			1635	731	296	530	76	2		

- Molecule 56 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	1y	74	Total	C	N	O	P	S	0	0
			1585	707	285	518	74	1		
56	2y	73	Total	C	N	O	P	S	0	0
			1565	698	283	510	73	1		

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1A	1108	Total	Mg	0	0
			1108	1108		
57	1B	36	Total	Mg	0	0
			36	36		
57	1D	12	Total	Mg	0	0
			12	12		
57	1E	16	Total	Mg	0	0
			16	16		
57	1F	12	Total	Mg	0	0
			12	12		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1G	5	Total 5	Mg 5	0	0
57	1I	1	Total 1	Mg 1	0	0
57	1N	6	Total 6	Mg 6	0	0
57	1O	6	Total 6	Mg 6	0	0
57	1P	6	Total 6	Mg 6	0	0
57	1Q	6	Total 6	Mg 6	0	0
57	1R	4	Total 4	Mg 4	0	0
57	1S	3	Total 3	Mg 3	0	0
57	1T	2	Total 2	Mg 2	0	0
57	1U	9	Total 9	Mg 9	0	0
57	1V	6	Total 6	Mg 6	0	0
57	1W	6	Total 6	Mg 6	0	0
57	1X	5	Total 5	Mg 5	0	0
57	1Y	4	Total 4	Mg 4	0	0
57	1Z	3	Total 3	Mg 3	0	0
57	10	8	Total 8	Mg 8	0	0
57	11	5	Total 5	Mg 5	0	0
57	12	2	Total 2	Mg 2	0	0
57	13	4	Total 4	Mg 4	0	0
57	14	1	Total 1	Mg 1	0	0
57	15	9	Total 9	Mg 9	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	16	1	Total 1	Mg 1	0	0
57	17	6	Total 6	Mg 6	0	0
57	18	6	Total 6	Mg 6	0	0
57	19	1	Total 1	Mg 1	0	0
57	1a	229	Total 229	Mg 229	0	0
57	1b	2	Total 2	Mg 2	0	0
57	1d	1	Total 1	Mg 1	0	0
57	1e	2	Total 2	Mg 2	0	0
57	1f	1	Total 1	Mg 1	0	0
57	1l	3	Total 3	Mg 3	0	0
57	1m	1	Total 1	Mg 1	0	0
57	1n	2	Total 2	Mg 2	0	0
57	1r	1	Total 1	Mg 1	0	0
57	1t	1	Total 1	Mg 1	0	0
57	1v	1	Total 1	Mg 1	0	0
57	1w	5	Total 5	Mg 5	0	0
57	1x	15	Total 15	Mg 15	0	0
57	1y	4	Total 4	Mg 4	0	0
57	2A	729	Total 729	Mg 729	0	0
57	2B	18	Total 18	Mg 18	0	0
57	2D	6	Total 6	Mg 6	0	0

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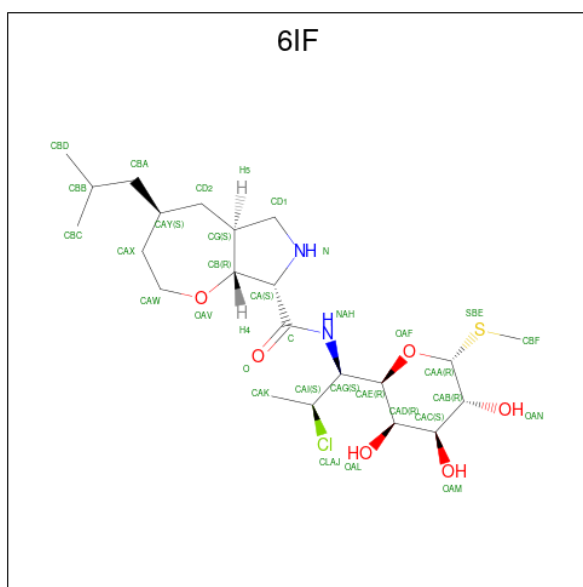
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	2E	7	Total 7	Mg 7	0	0
57	2F	6	Total 6	Mg 6	0	0
57	2G	1	Total 1	Mg 1	0	0
57	2N	1	Total 1	Mg 1	0	0
57	2O	1	Total 1	Mg 1	0	0
57	2Q	1	Total 1	Mg 1	0	0
57	2R	1	Total 1	Mg 1	0	0
57	2T	3	Total 3	Mg 3	0	0
57	2W	1	Total 1	Mg 1	0	0
57	2X	1	Total 1	Mg 1	0	0
57	2Y	1	Total 1	Mg 1	0	0
57	2Z	1	Total 1	Mg 1	0	0
57	20	3	Total 3	Mg 3	0	0
57	21	1	Total 1	Mg 1	0	0
57	23	2	Total 2	Mg 2	0	0
57	25	3	Total 3	Mg 3	0	0
57	26	1	Total 1	Mg 1	0	0
57	27	3	Total 3	Mg 3	0	0
57	28	3	Total 3	Mg 3	0	0
57	2a	186	Total 186	Mg 186	0	0
57	2d	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	2e	1	Total Mg 1 1	0	0
57	2f	2	Total Mg 2 2	0	0
57	2l	3	Total Mg 3 3	0	0
57	2q	3	Total Mg 3 3	0	0
57	2r	1	Total Mg 1 1	0	0
57	2t	1	Total Mg 1 1	0	0
57	2v	1	Total Mg 1 1	0	0
57	2w	1	Total Mg 1 1	0	0
57	2x	5	Total Mg 5 5	0	0
57	2y	3	Total Mg 3 3	0	0

- Molecule 58 is methyl 7-chloro-6,7,8-trideoxy-6-{[(4S,5aS,8S,8aR)-4-(2-methylpropyl)octahydro-2H-oxepino[2,3-c]pyrrole-8-carbonyl]amino}-1-thio-L-threo- α -D-galacto-octopyranoside (three-letter code: 6IF) (formula: C₂₂H₃₉ClN₂O₆S).

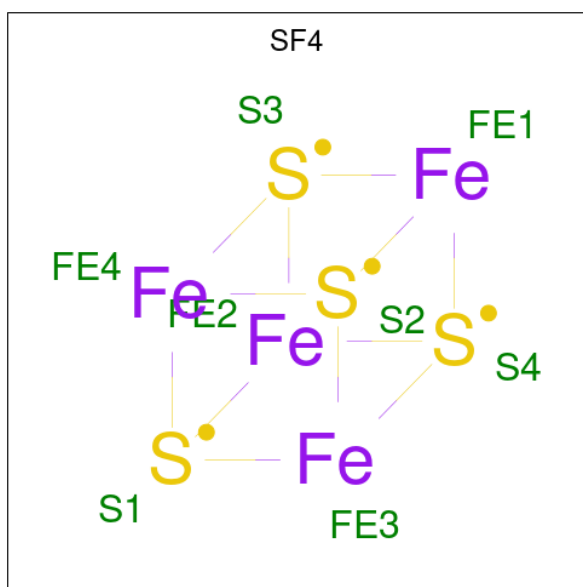


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
58	1A	1	Total	C	Cl	N	O	S	0	0
			32	22	1	2	6	1		
58	2A	1	Total	C	Cl	N	O	S	0	0
			32	22	1	2	6	1		

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1Y	1	Total	Zn	0	0
			1	1		
59	14	1	Total	Zn	0	0
			1	1		
59	15	1	Total	Zn	0	0
			1	1		
59	16	1	Total	Zn	0	0
			1	1		
59	19	1	Total	Zn	0	0
			1	1		
59	1n	1	Total	Zn	0	0
			1	1		
59	2Y	1	Total	Zn	0	0
			1	1		
59	24	1	Total	Zn	0	0
			1	1		
59	25	1	Total	Zn	0	0
			1	1		
59	26	1	Total	Zn	0	0
			1	1		
59	29	1	Total	Zn	0	0
			1	1		
59	2n	1	Total	Zn	0	0
			1	1		

- Molecule 60 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
60	1d	1	Total	Fe	S	0	0
			8	4	4		
60	2d	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 61 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2A	1	Total	K	0	0
			1	1		

- Molecule 62 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	1A	2122	Total	O	0	0
			2122	2122		
62	1B	69	Total	O	0	0
			69	69		
62	1D	24	Total	O	0	0
			24	24		
62	1E	27	Total	O	0	0
			27	27		
62	1F	18	Total	O	0	0
			18	18		
62	1G	7	Total	O	0	0
			7	7		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	1H	2	Total	O	0	0
			2	2		
62	1N	4	Total	O	0	0
			4	4		
62	1O	7	Total	O	0	0
			7	7		
62	1P	20	Total	O	0	0
			20	20		
62	1Q	8	Total	O	0	0
			8	8		
62	1R	10	Total	O	0	0
			10	10		
62	1S	4	Total	O	0	0
			4	4		
62	1T	8	Total	O	0	0
			8	8		
62	1U	10	Total	O	0	0
			10	10		
62	1V	9	Total	O	0	0
			9	9		
62	1W	7	Total	O	0	0
			7	7		
62	1X	7	Total	O	0	0
			7	7		
62	1Y	3	Total	O	0	0
			3	3		
62	1Z	1	Total	O	0	0
			1	1		
62	10	10	Total	O	0	0
			10	10		
62	11	12	Total	O	0	0
			12	12		
62	12	4	Total	O	0	0
			4	4		
62	13	5	Total	O	0	0
			5	5		
62	15	7	Total	O	0	0
			7	7		
62	16	1	Total	O	0	0
			1	1		
62	17	8	Total	O	0	0
			8	8		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	18	10	Total 10	O 10	0	0
62	1a	361	Total 361	O 361	0	0
62	1b	1	Total 1	O 1	0	0
62	1d	1	Total 1	O 1	0	0
62	1e	1	Total 1	O 1	0	0
62	1g	1	Total 1	O 1	0	0
62	1l	4	Total 4	O 4	0	0
62	1m	2	Total 2	O 2	0	0
62	1q	4	Total 4	O 4	0	0
62	1u	1	Total 1	O 1	0	0
62	1v	5	Total 5	O 5	0	0
62	1w	6	Total 6	O 6	0	0
62	1x	16	Total 16	O 16	0	0
62	1y	2	Total 2	O 2	0	0
62	2A	968	Total 968	O 968	0	0
62	2B	15	Total 15	O 15	0	0
62	2D	16	Total 16	O 16	0	0
62	2E	9	Total 9	O 9	0	0
62	2F	9	Total 9	O 9	0	0
62	2I	1	Total 1	O 1	0	0
62	2N	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	2O	2	Total 2	O 2	0	0
62	2P	10	Total 10	O 10	0	0
62	2Q	1	Total 1	O 1	0	0
62	2R	3	Total 3	O 3	0	0
62	2T	2	Total 2	O 2	0	0
62	2W	1	Total 1	O 1	0	0
62	2X	3	Total 3	O 3	0	0
62	2Y	1	Total 1	O 1	0	0
62	20	2	Total 2	O 2	0	0
62	21	3	Total 3	O 3	0	0
62	23	2	Total 2	O 2	0	0
62	25	2	Total 2	O 2	0	0
62	26	1	Total 1	O 1	0	0
62	27	2	Total 2	O 2	0	0
62	28	6	Total 6	O 6	0	0
62	29	1	Total 1	O 1	0	0
62	2a	51	Total 51	O 51	0	0
62	2d	1	Total 1	O 1	0	0
62	2i	1	Total 1	O 1	0	0
62	2j	1	Total 1	O 1	0	0
62	2l	3	Total 3	O 3	0	0

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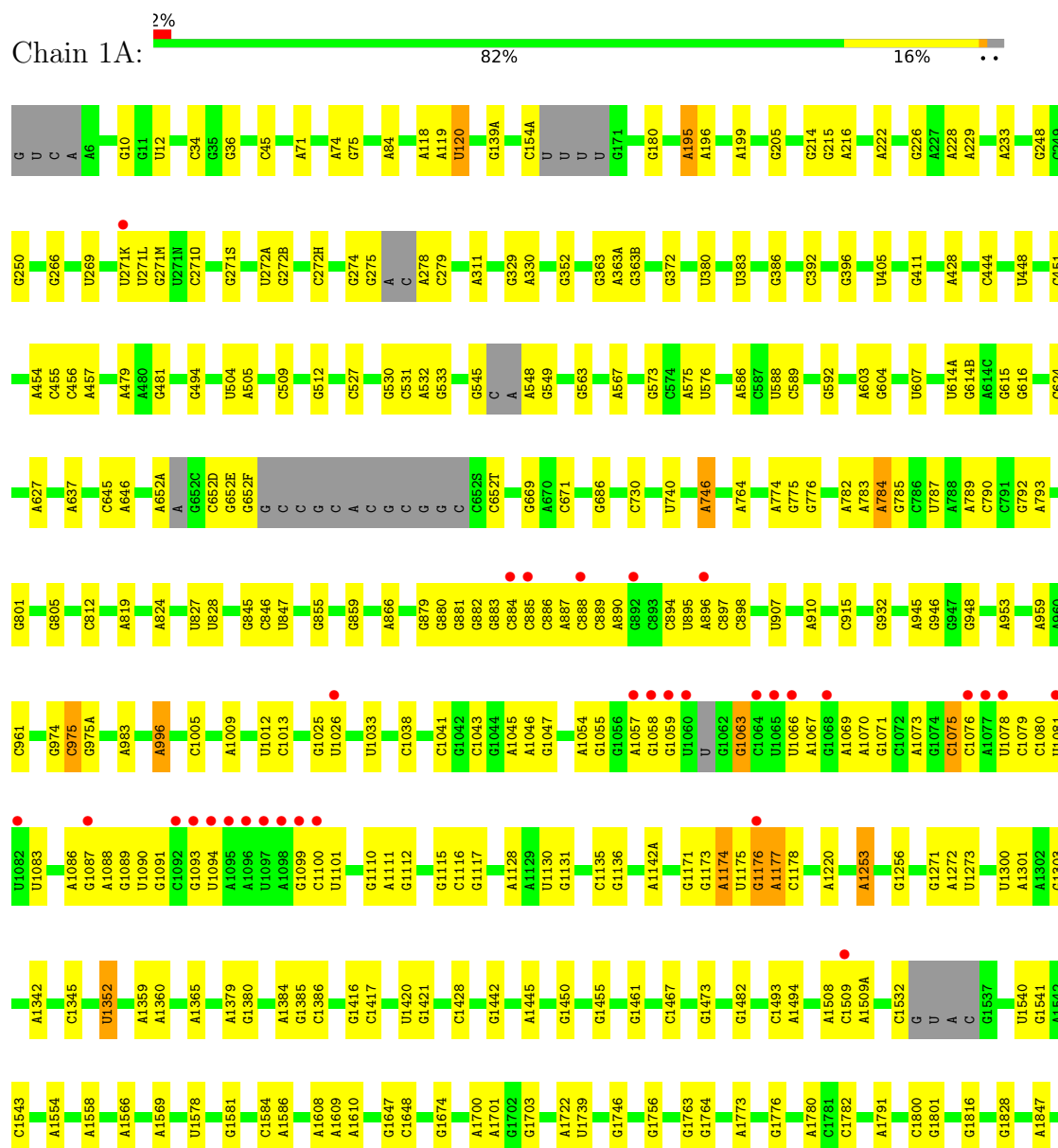
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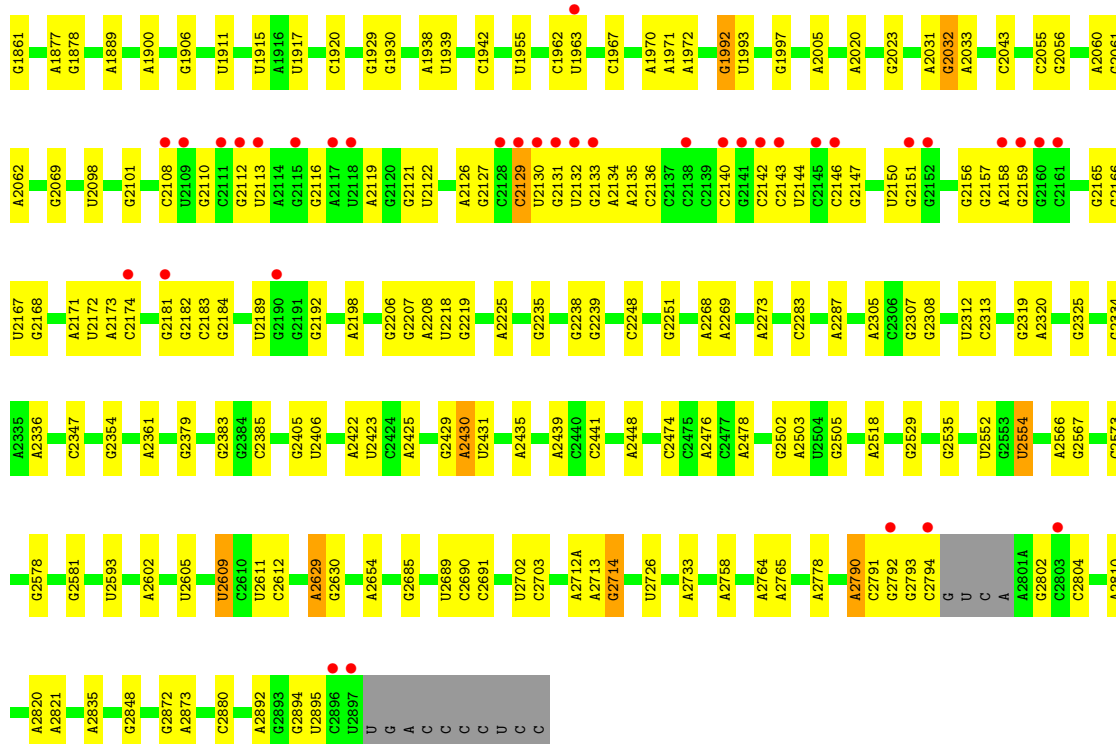
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62	2p	1	Total 1	O 1	0	0
62	2t	2	Total 2	O 2	0	0
62	2x	3	Total 3	O 3	0	0
62	2y	8	Total 8	O 8	0	0

3 Residue-property plots [i](#)

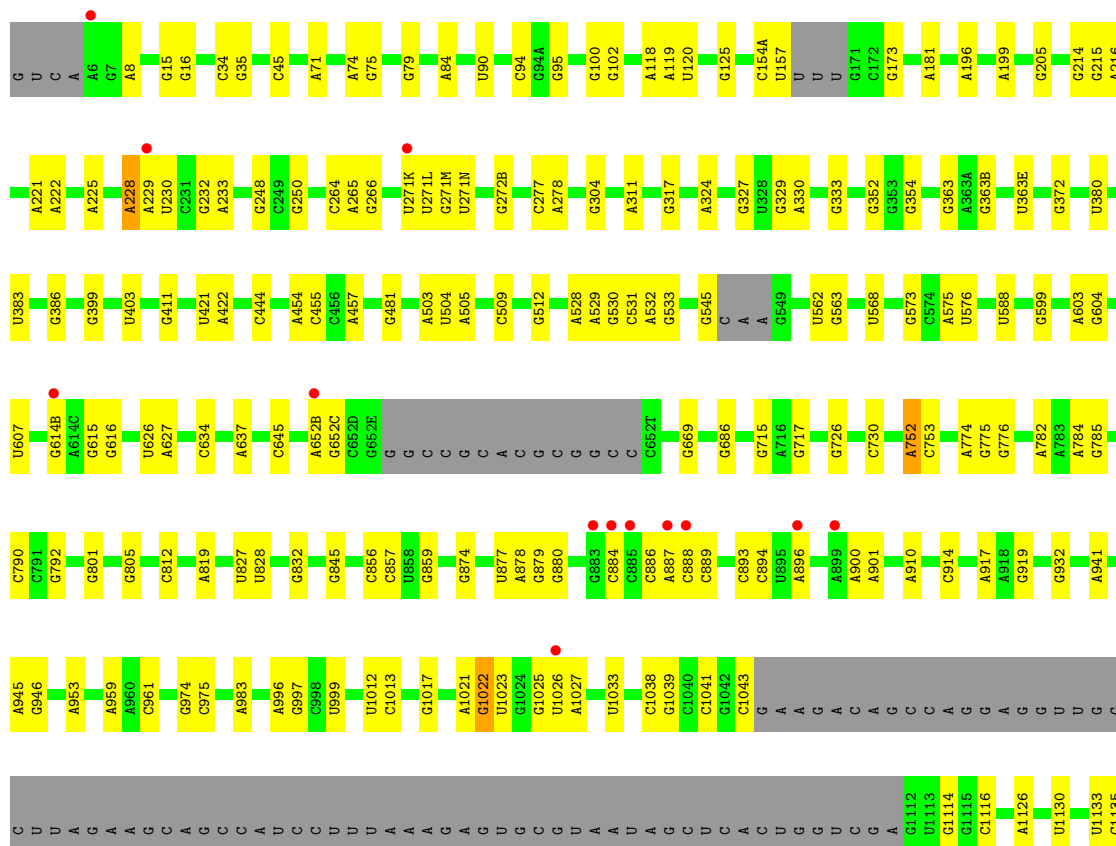
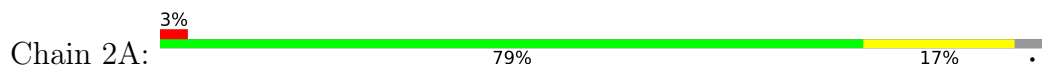
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

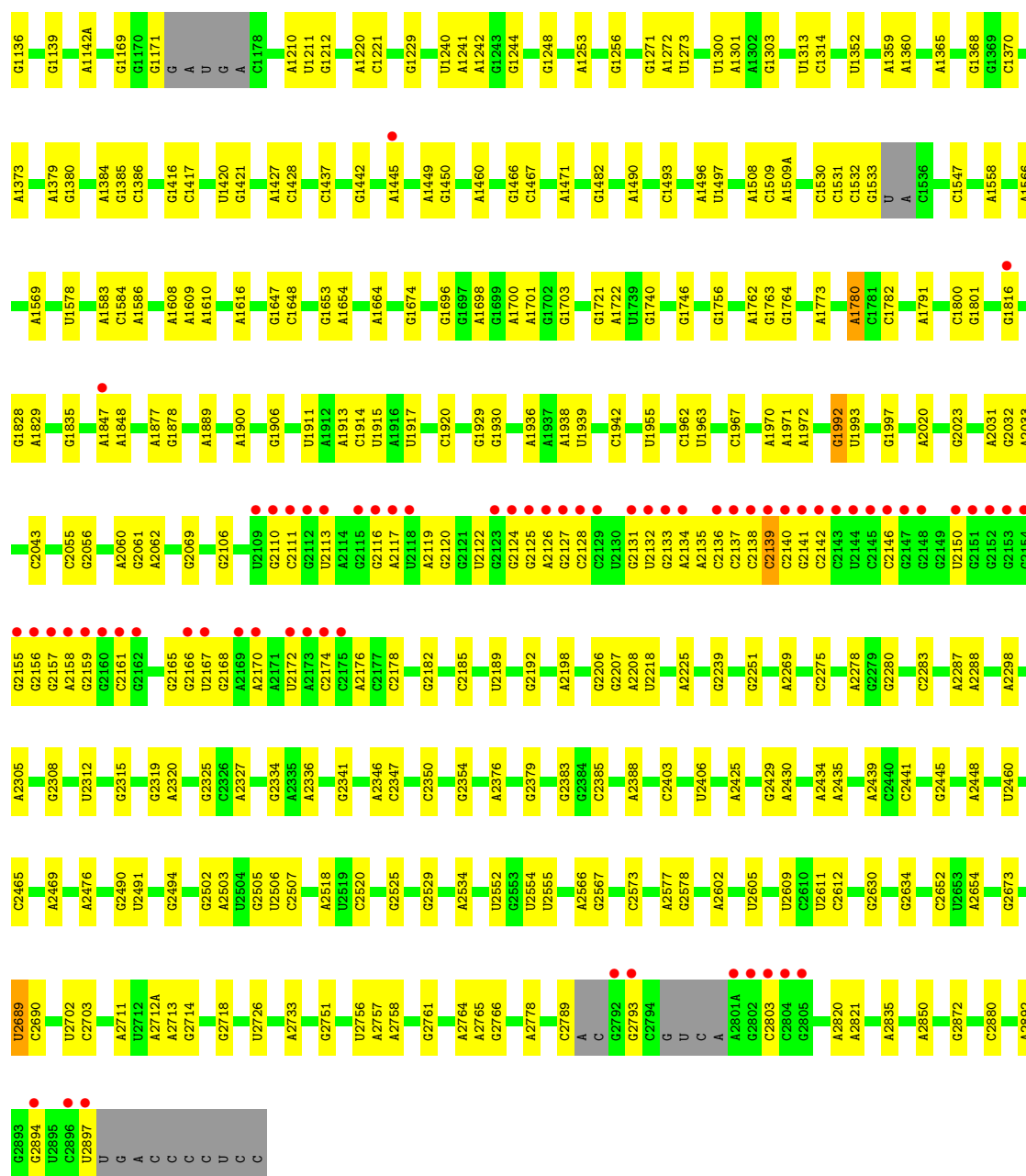
• Molecule 1: 23S Ribosomal RNA



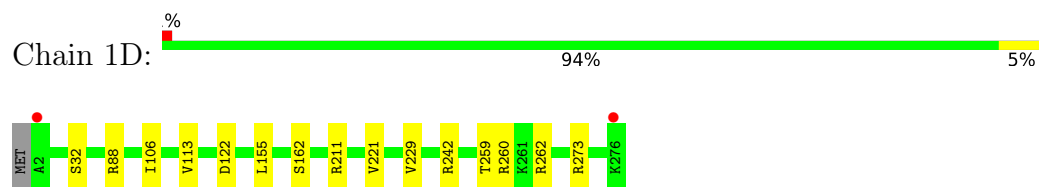


• Molecule 1: 23S Ribosomal RNA

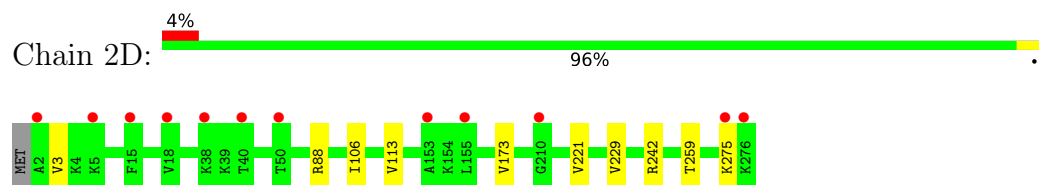




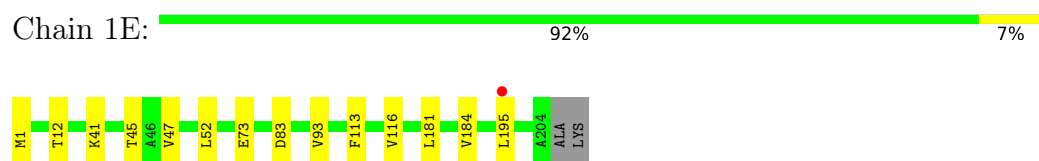
- Molecule 3: 50S ribosomal protein L2



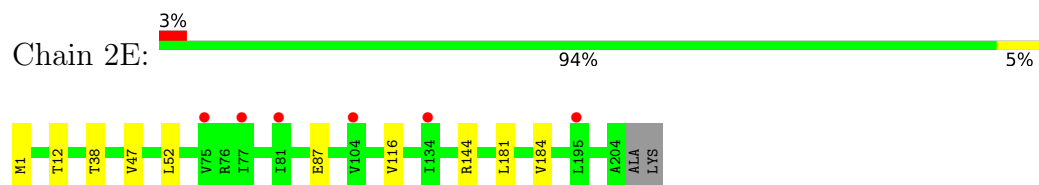
- Molecule 3: 50S ribosomal protein L2



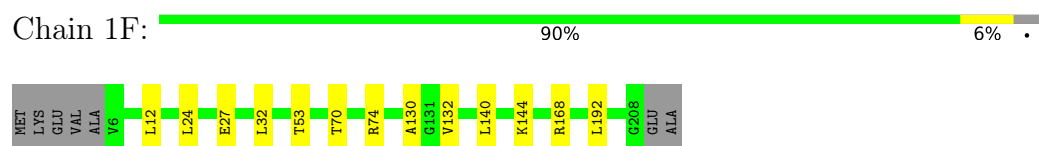
- Molecule 4: 50S ribosomal protein L3



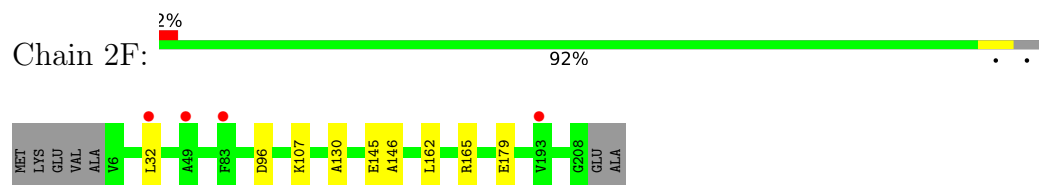
- Molecule 4: 50S ribosomal protein L3



- Molecule 5: 50S ribosomal protein L4

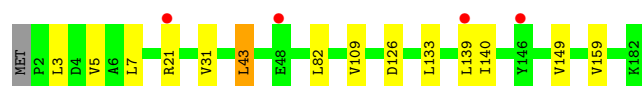


- Molecule 5: 50S ribosomal protein L4

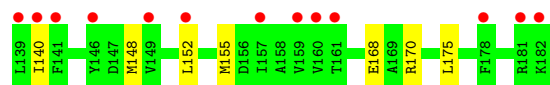
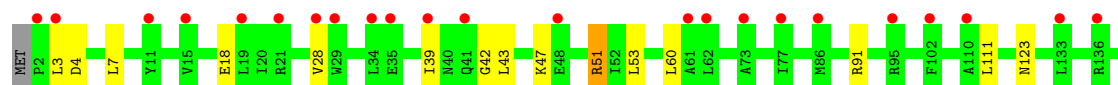
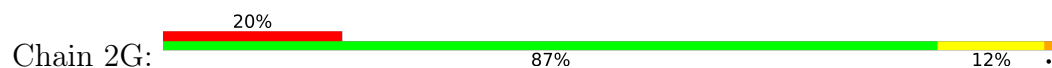


- Molecule 6: 50S ribosomal protein L5





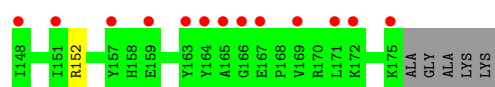
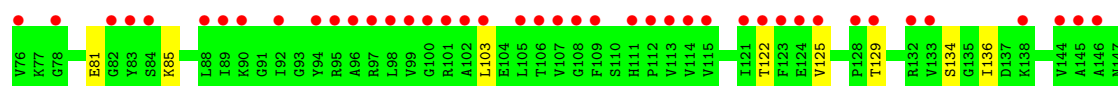
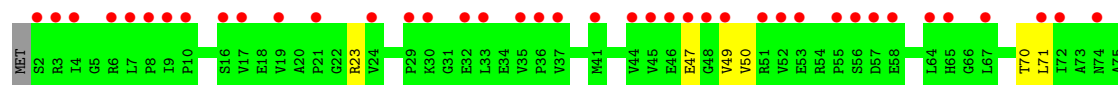
- Molecule 6: 50S ribosomal protein L5



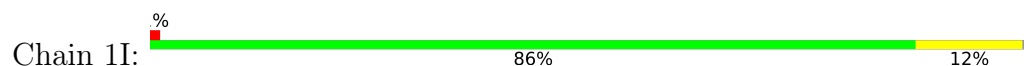
- Molecule 7: 50S ribosomal protein L6



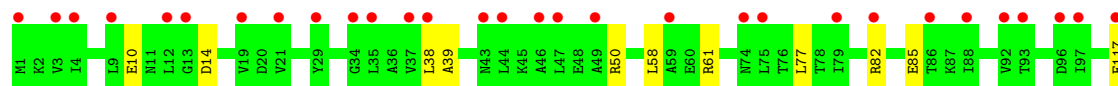
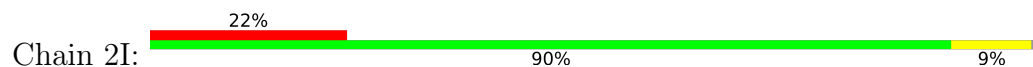
- Molecule 7: 50S ribosomal protein L6

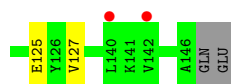


- Molecule 8: 50S ribosomal protein L9



- Molecule 8: 50S ribosomal protein L9





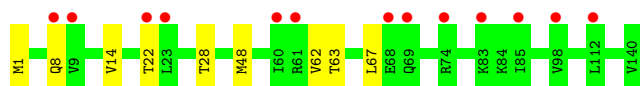
- Molecule 9: 50S ribosomal protein L13

Chain 1N: 95% 5%



- Molecule 9: 50S ribosomal protein L13

Chain 2N: 9% 94% 6%



- Molecule 10: 50S ribosomal protein L14

Chain 1O: 0% 98% 2%



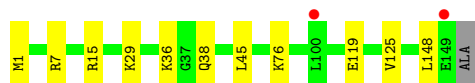
- Molecule 10: 50S ribosomal protein L14

Chain 2O: 7% 97% 3%



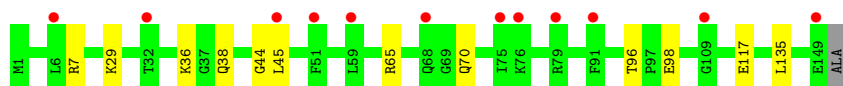
- Molecule 11: 50S ribosomal protein L15

Chain 1P: 0% 92% 7%



- Molecule 11: 50S ribosomal protein L15

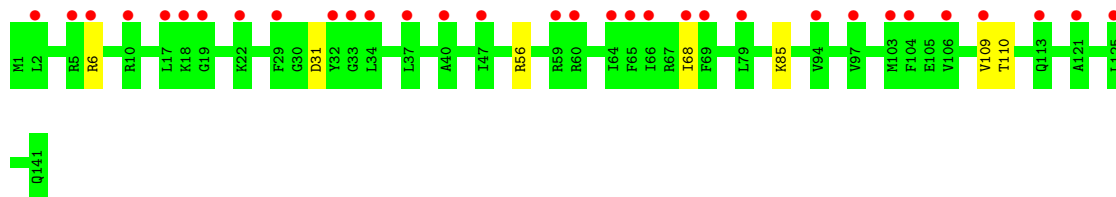
Chain 2P: 8% 91% 8%



- Molecule 12: 50S ribosomal protein L16



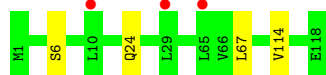
- Molecule 12: 50S ribosomal protein L16



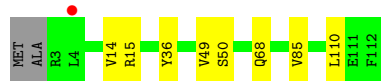
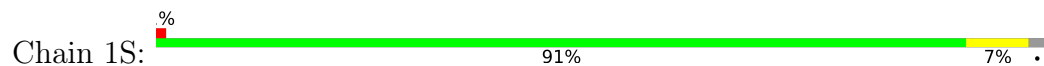
- Molecule 13: 50S ribosomal protein L17



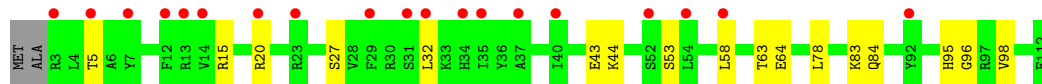
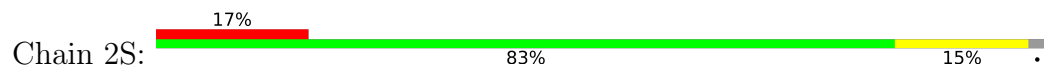
- Molecule 13: 50S ribosomal protein L17



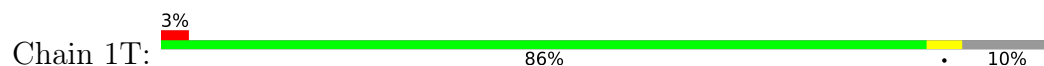
- Molecule 14: 50S ribosomal protein L18

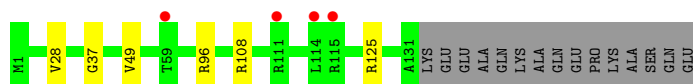


- Molecule 14: 50S ribosomal protein L18

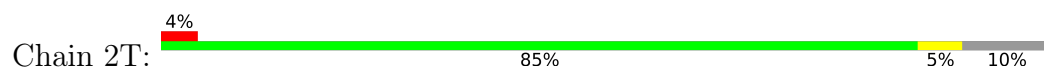


- Molecule 15: 50S ribosomal protein L19

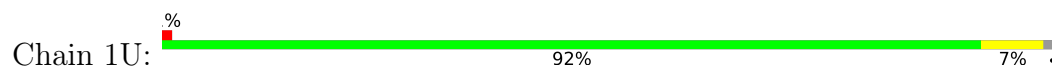




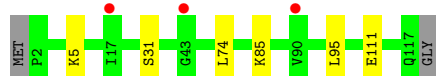
- Molecule 15: 50S ribosomal protein L19



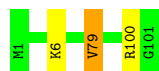
- Molecule 16: 50S ribosomal protein L20



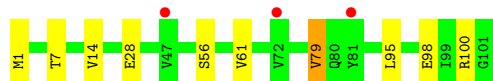
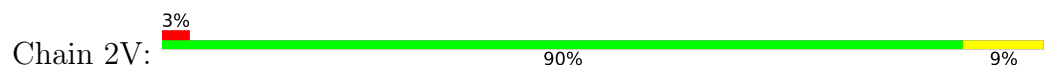
- Molecule 16: 50S ribosomal protein L20



- Molecule 17: 50S ribosomal protein L21



- Molecule 17: 50S ribosomal protein L21



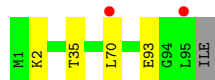
- Molecule 18: 50S ribosomal protein L22



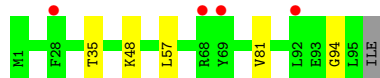
- Molecule 18: 50S ribosomal protein L22



- Molecule 19: 50S ribosomal protein L23



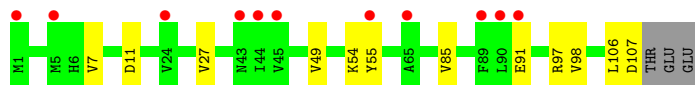
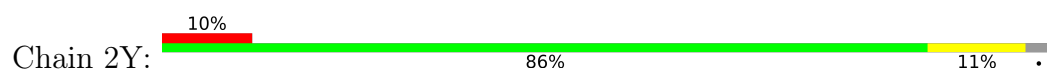
- Molecule 19: 50S ribosomal protein L23



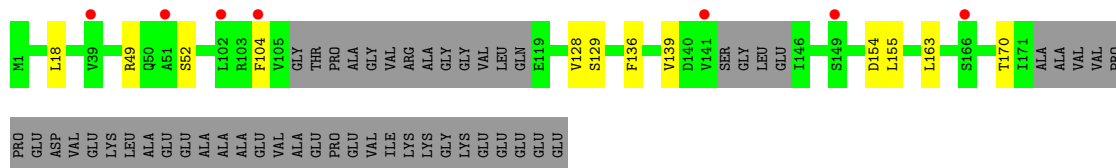
- Molecule 20: 50S ribosomal protein L24



- Molecule 20: 50S ribosomal protein L24

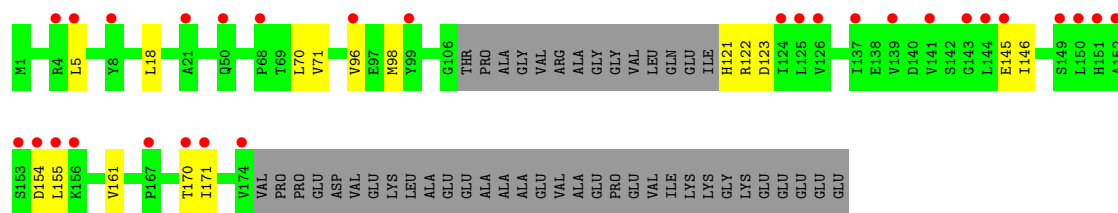


- Molecule 21: 50S ribosomal protein L25

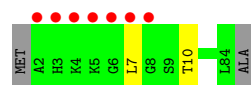


- Molecule 21: 50S ribosomal protein L25

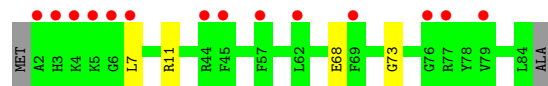




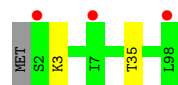
- Molecule 22: 50S ribosomal protein L27



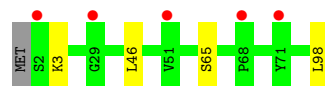
- Molecule 22: 50S ribosomal protein L27



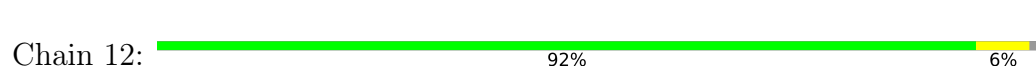
- Molecule 23: 50S ribosomal protein L28



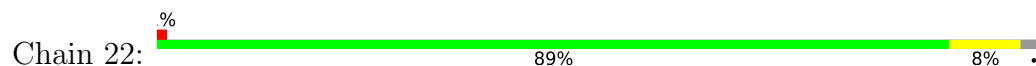
- Molecule 23: 50S ribosomal protein L28



- Molecule 24: 50S ribosomal protein L29



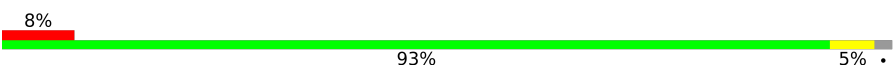
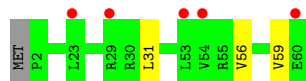
- Molecule 24: 50S ribosomal protein L29




• Molecule 25: 50S ribosomal protein L30

Chain 13:  92% 7% .


• Molecule 25: 50S ribosomal protein L30

Chain 23:  8% 93% 5% .

• Molecule 26: 50S ribosomal protein L31

Chain 14:  4% 83% 10% . .

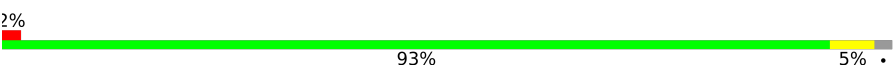
• Molecule 26: 50S ribosomal protein L31

Chain 24:  21% 77% 18% . .

• Molecule 27: 50S ribosomal protein L32

Chain 15:  2% 95% . .

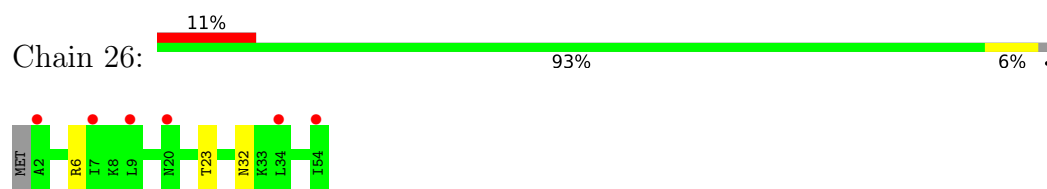
• Molecule 27: 50S ribosomal protein L32

Chain 25:  2% 93% 5% .

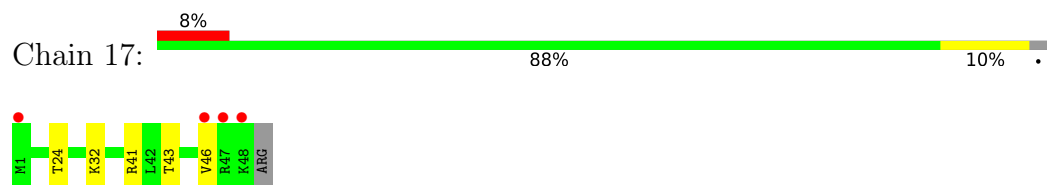
• Molecule 28: 50S ribosomal protein L33

Chain 16:  91% 7% .

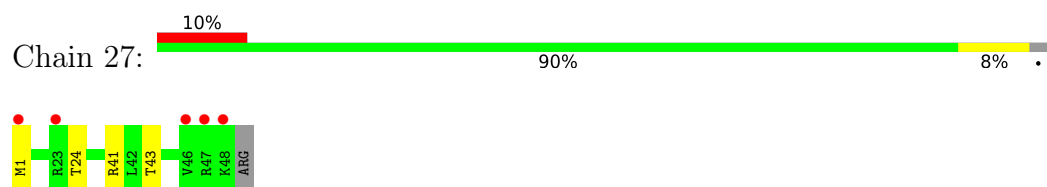
- Molecule 28: 50S ribosomal protein L33



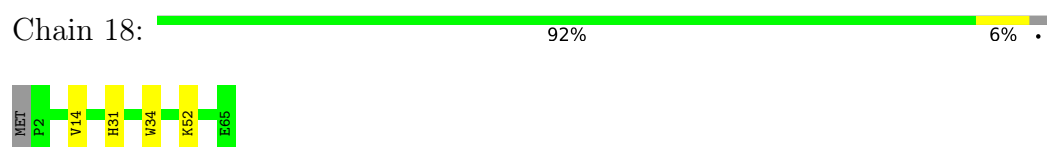
- Molecule 29: 50S ribosomal protein L34



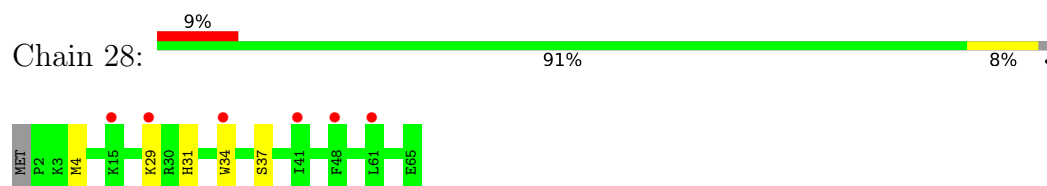
- Molecule 29: 50S ribosomal protein L34



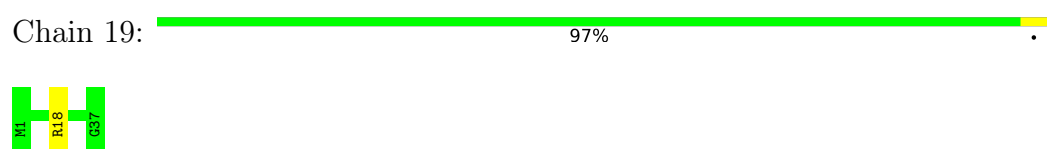
- Molecule 30: 50S ribosomal protein L35



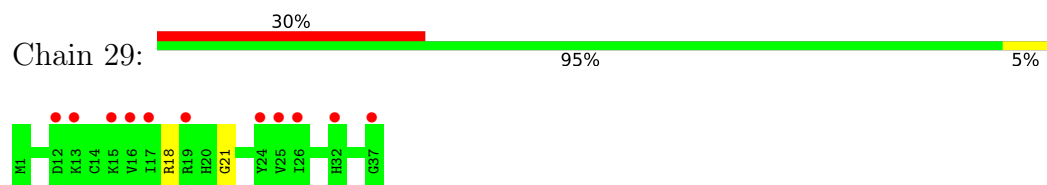
- Molecule 30: 50S ribosomal protein L35



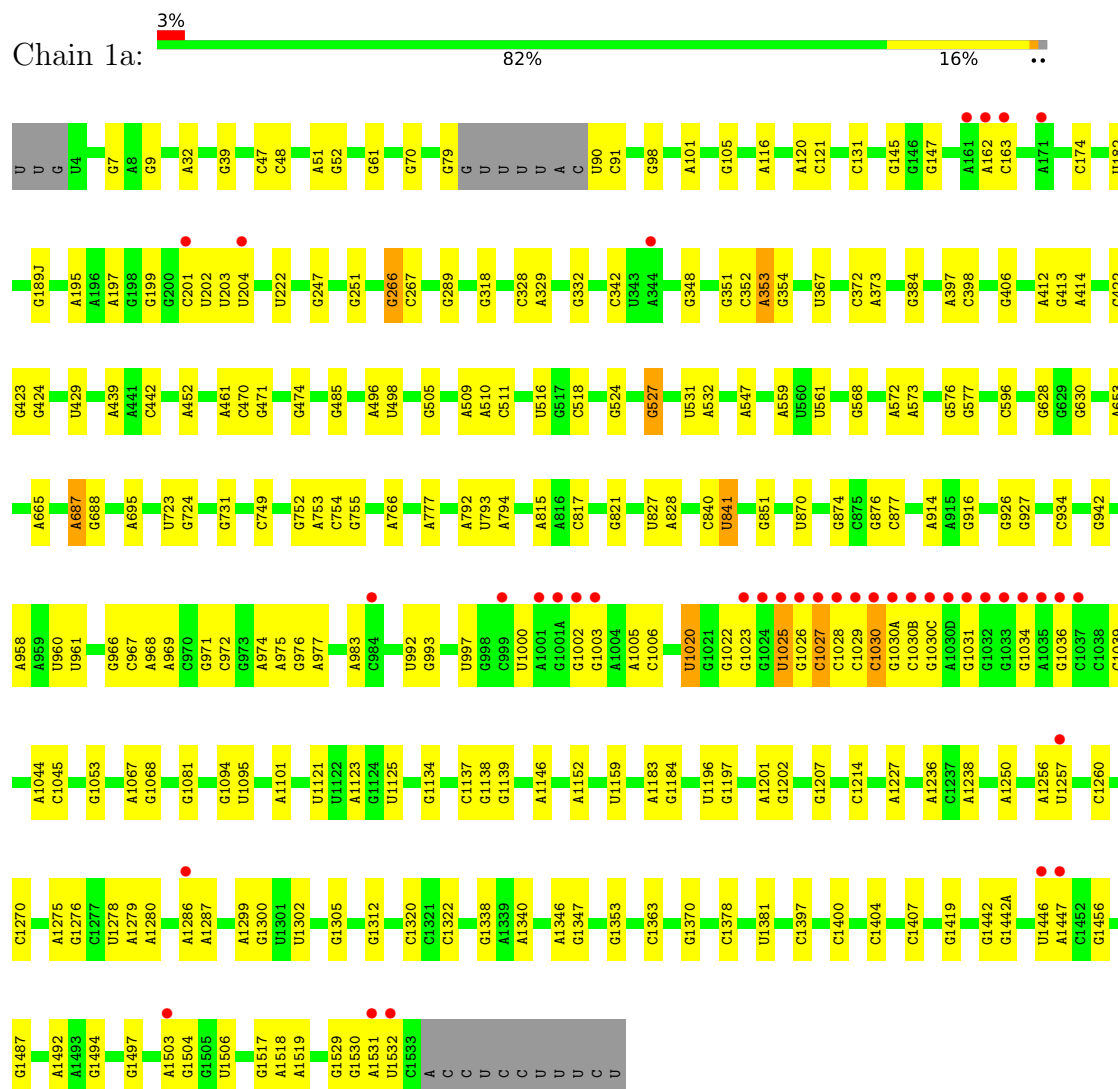
- Molecule 31: 50S ribosomal protein L36



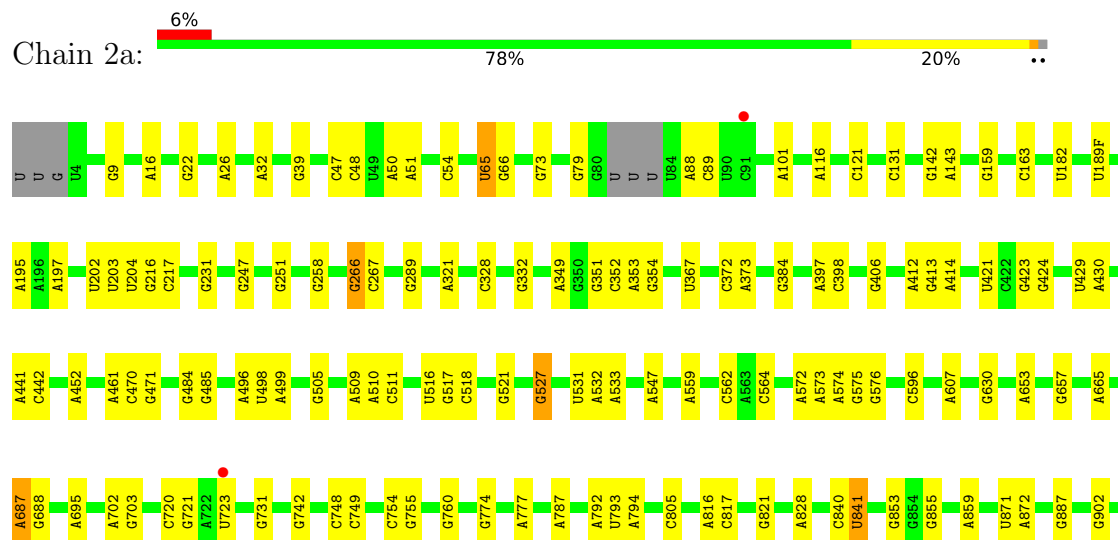
- Molecule 31: 50S ribosomal protein L36

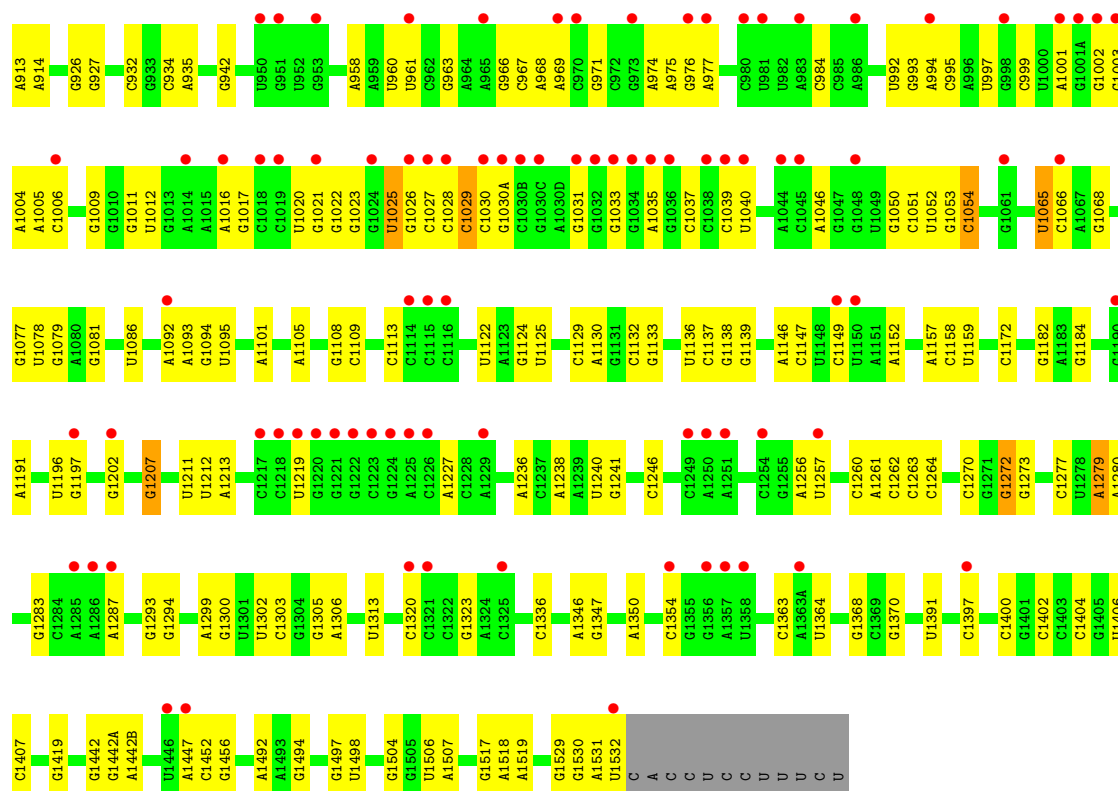


- Molecule 32: 16S Ribosomal RNA

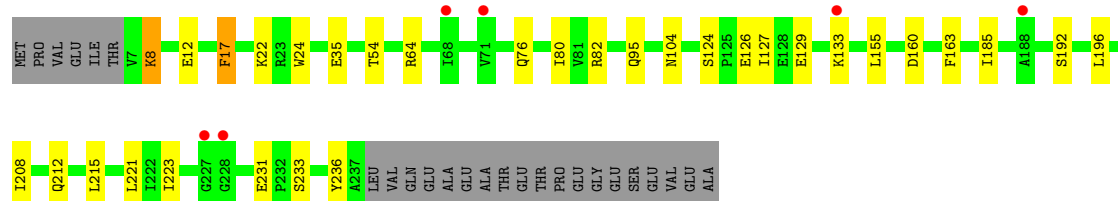
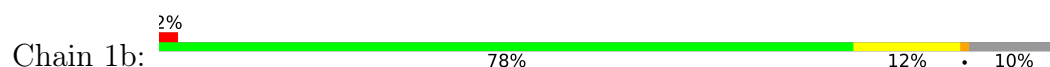


- Molecule 32: 16S Ribosomal RNA

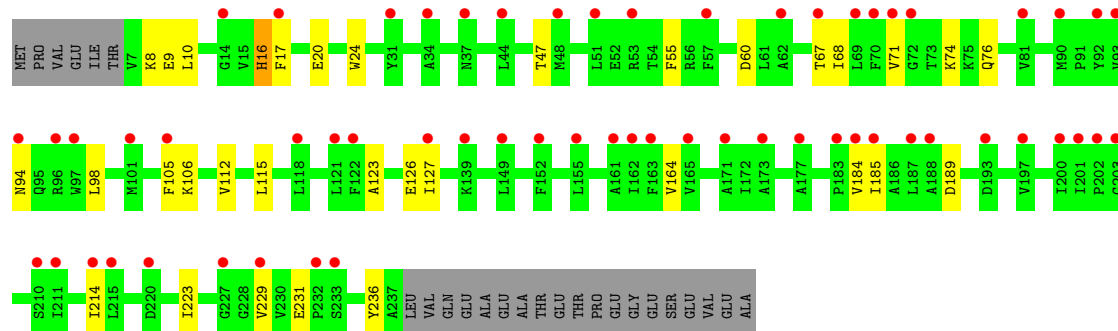
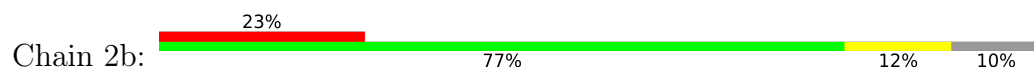




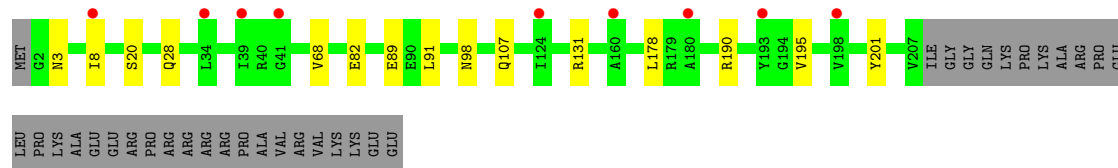
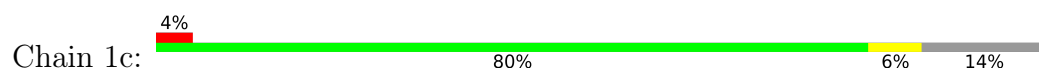
- Molecule 33: 30S ribosomal protein S2



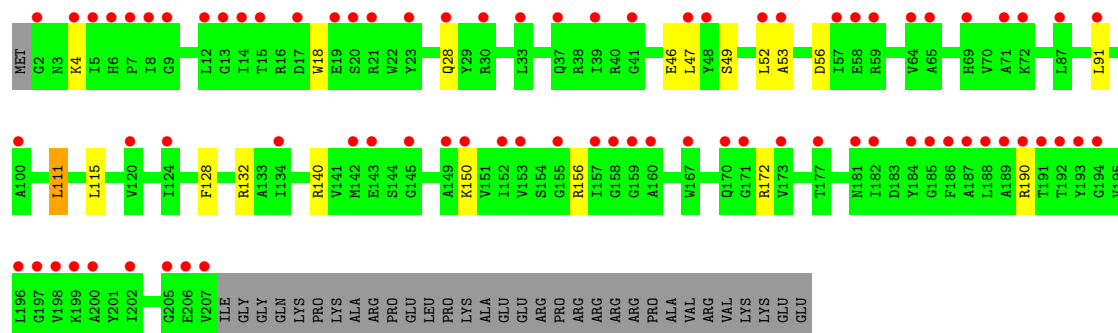
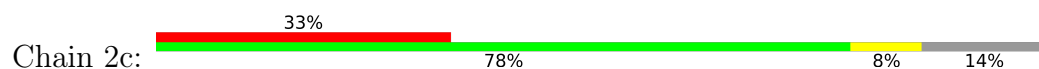
- Molecule 33: 30S ribosomal protein S2



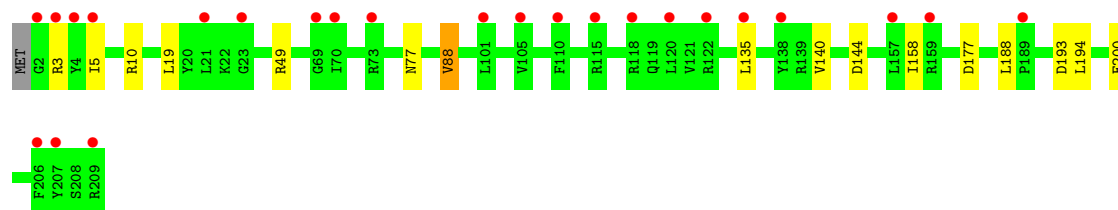
- Molecule 34: 30S ribosomal protein S3



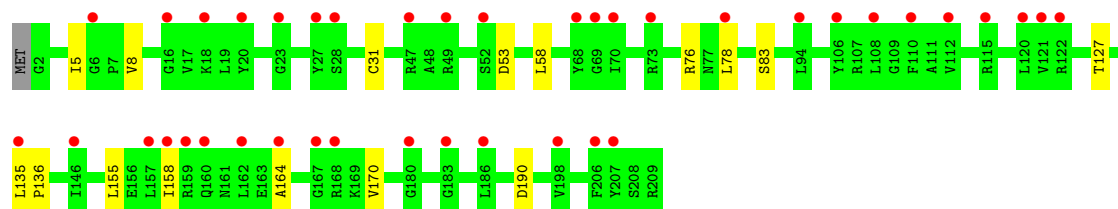
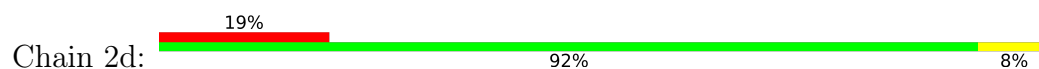
• Molecule 34: 30S ribosomal protein S3



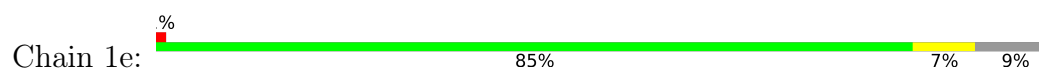
• Molecule 35: 30S ribosomal protein S4



• Molecule 35: 30S ribosomal protein S4

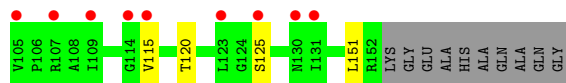
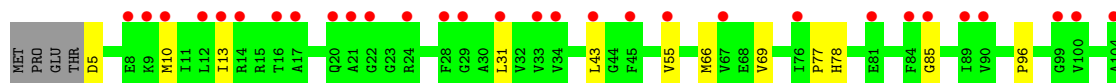
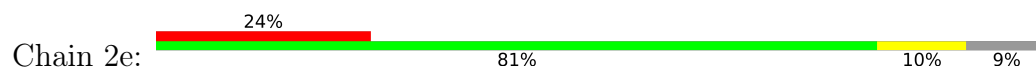


• Molecule 36: 30S ribosomal protein S5





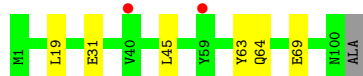
- Molecule 36: 30S ribosomal protein S5



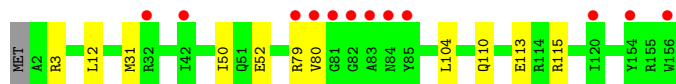
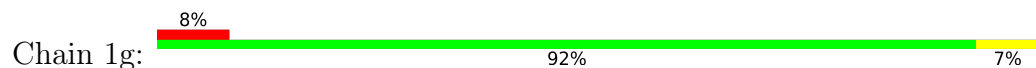
- Molecule 37: 30S ribosomal protein S6



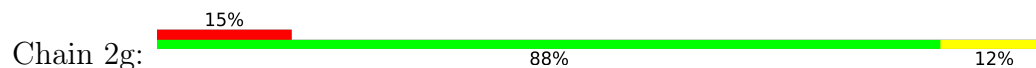
- Molecule 37: 30S ribosomal protein S6



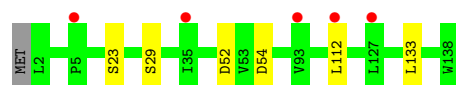
- Molecule 38: 30S ribosomal protein S7



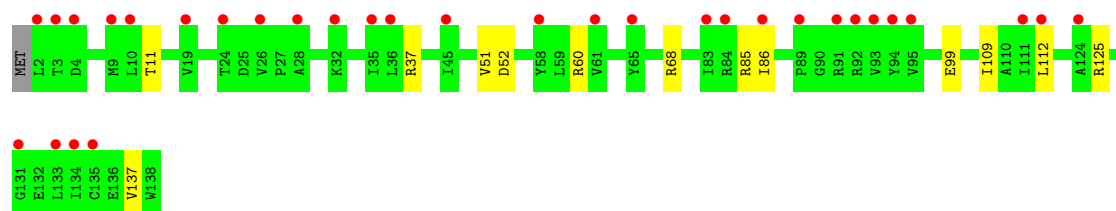
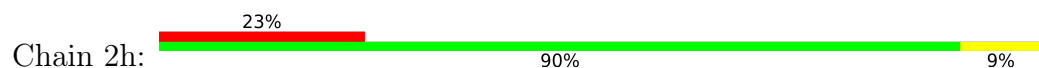
- Molecule 38: 30S ribosomal protein S7



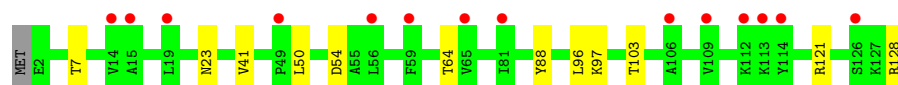
- Molecule 39: 30S ribosomal protein S8



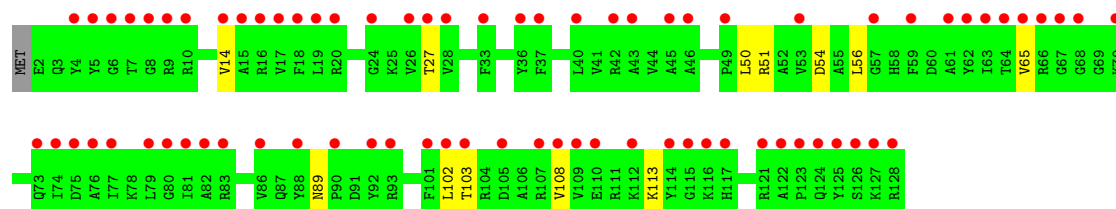
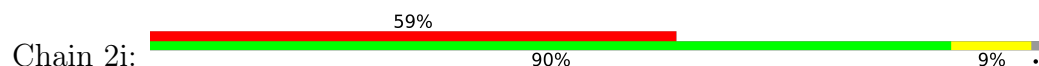
- Molecule 39: 30S ribosomal protein S8



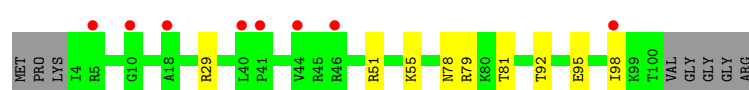
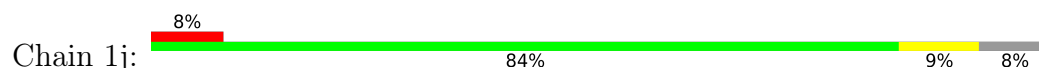
- Molecule 40: 30S ribosomal protein S9



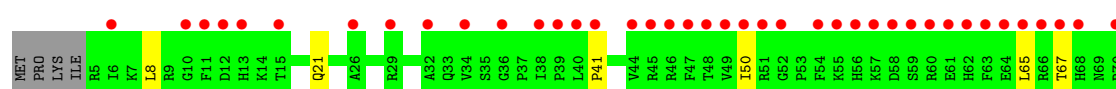
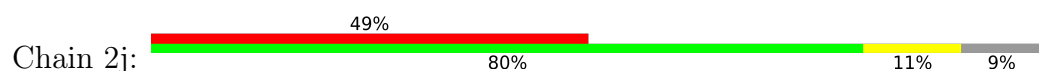
- Molecule 40: 30S ribosomal protein S9

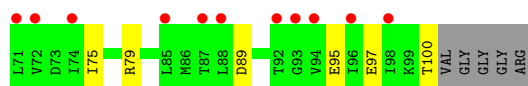


- Molecule 41: 30S ribosomal protein S10

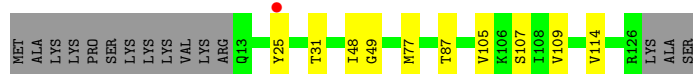
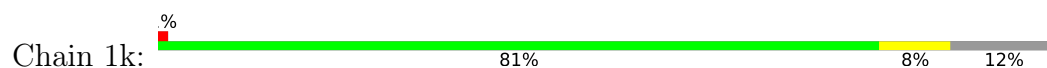


- Molecule 41: 30S ribosomal protein S10

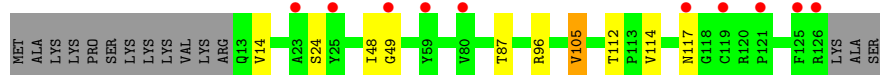
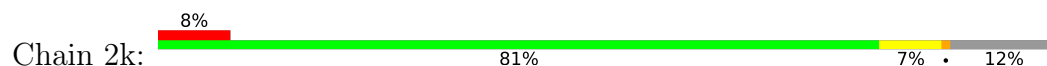




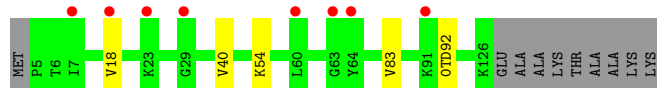
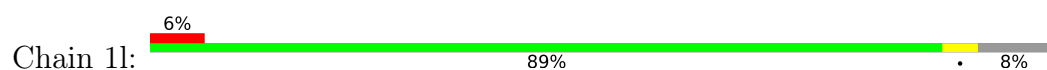
- Molecule 42: 30S ribosomal protein S11



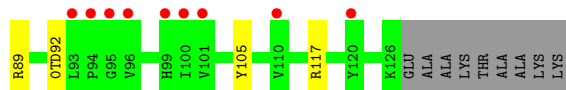
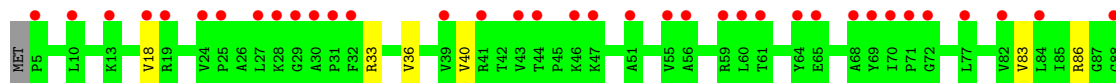
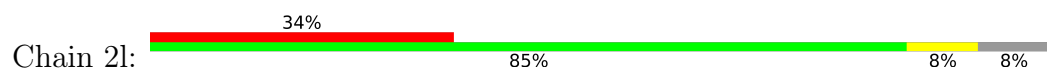
- Molecule 42: 30S ribosomal protein S11



- Molecule 43: 30S ribosomal protein S12



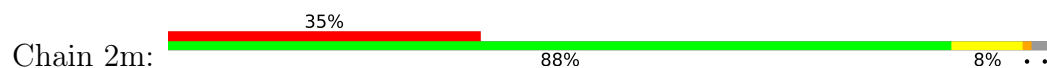
- Molecule 43: 30S ribosomal protein S12

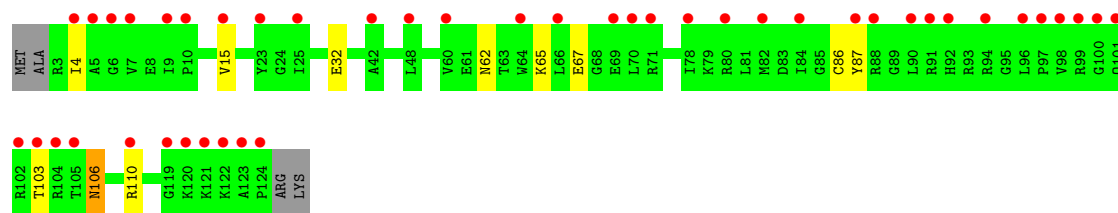


- Molecule 44: 30S ribosomal protein S13



- Molecule 44: 30S ribosomal protein S13

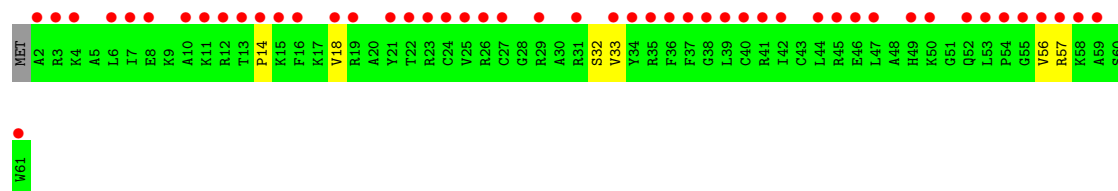
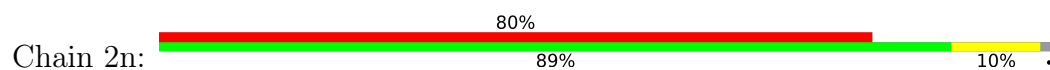




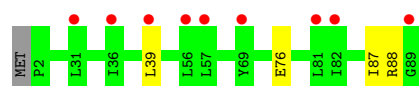
- Molecule 45: 30S ribosomal protein S14 type Z



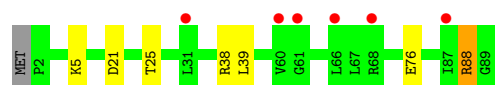
- Molecule 45: 30S ribosomal protein S14 type Z



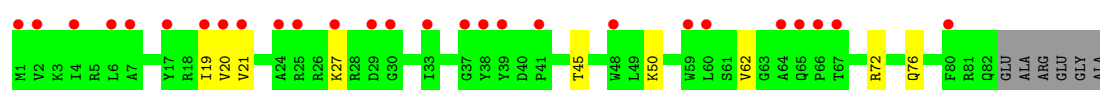
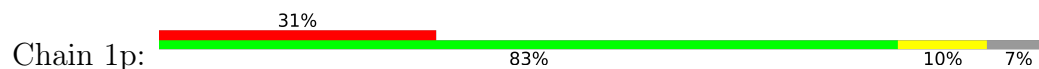
- Molecule 46: 30S ribosomal protein S15



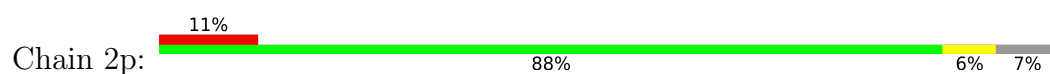
- Molecule 46: 30S ribosomal protein S15



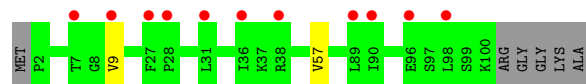
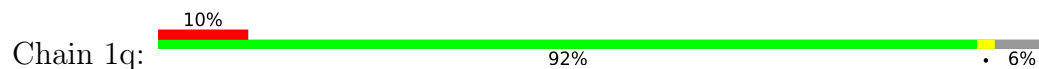
- Molecule 47: 30S ribosomal protein S16



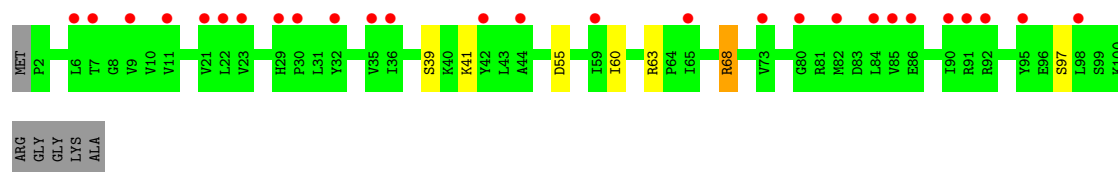
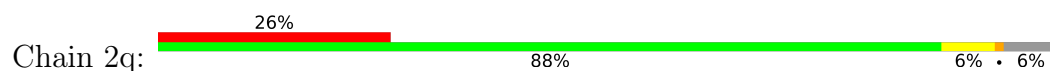
- Molecule 47: 30S ribosomal protein S16



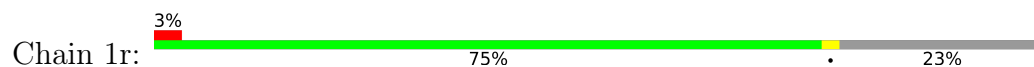
- Molecule 48: 30S ribosomal protein S17



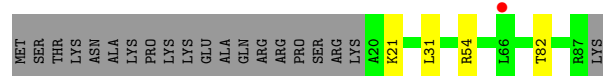
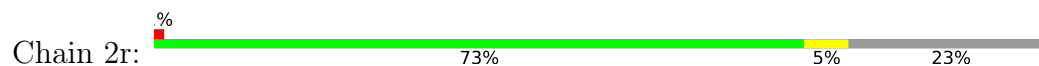
- Molecule 48: 30S ribosomal protein S17



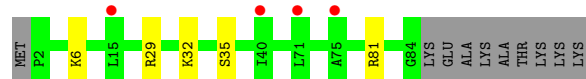
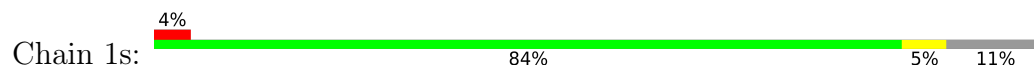
- Molecule 49: 30S ribosomal protein S18



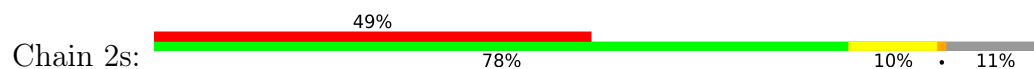
- Molecule 49: 30S ribosomal protein S18

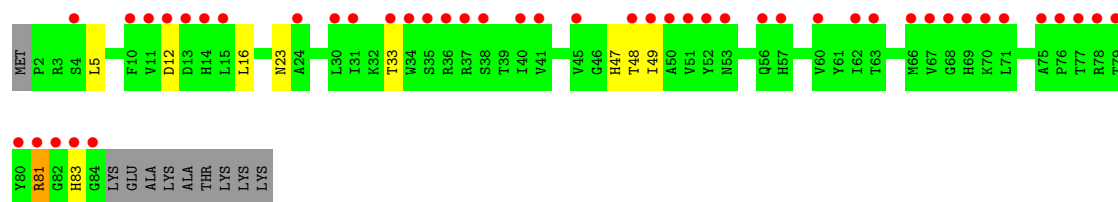


- Molecule 50: 30S ribosomal protein S19

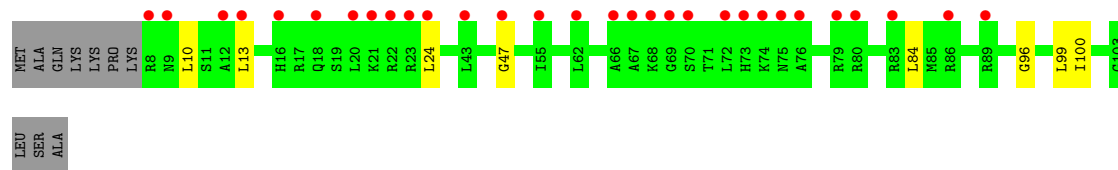
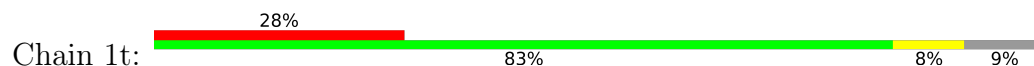


- Molecule 50: 30S ribosomal protein S19

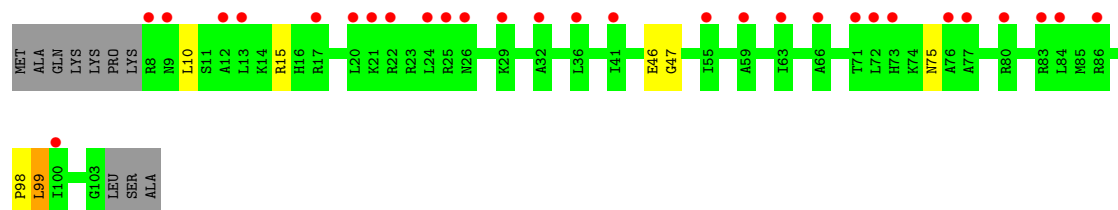
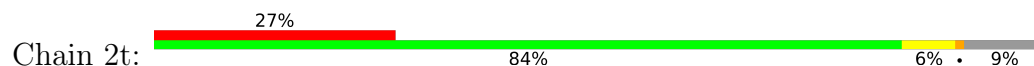




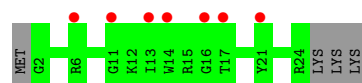
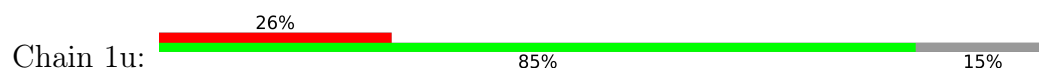
- Molecule 51: 30S ribosomal protein S20



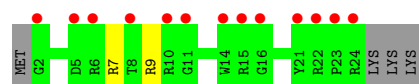
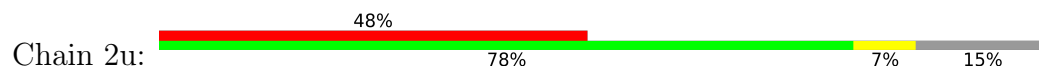
- Molecule 51: 30S ribosomal protein S20



- Molecule 52: 30S ribosomal protein Thx



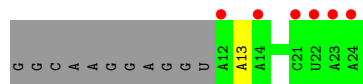
- Molecule 52: 30S ribosomal protein Thx



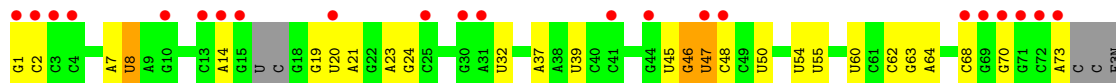
- Molecule 53: mRNA



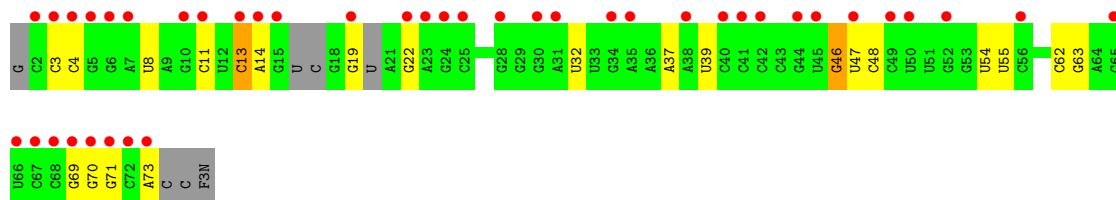
- Molecule 53: mRNA



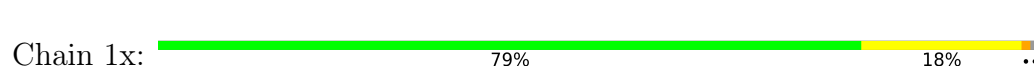
- Molecule 54: A-site tRNA



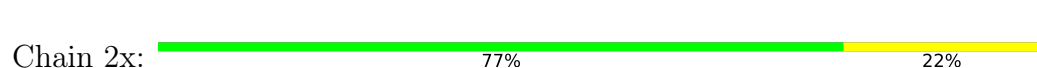
- Molecule 54: A-site tRNA



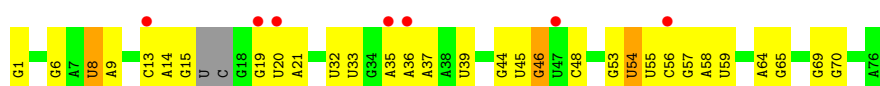
- Molecule 55: P-site tRNA



- Molecule 55: P-site tRNA

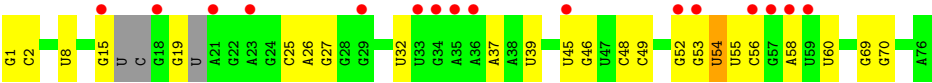


- Molecule 56: E-site tRNA



- Molecule 56: E-site tRNA





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.86Å 449.80Å 621.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	198.84 – 2.50 198.84 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (198.84-2.50) 99.8 (198.84-2.50)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 2.52Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.224 , 0.268 0.224 , 0.268	Depositor DCC
R_{free} test set	100061 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	51.2	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 53.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	299504	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.58% 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: MG, 5MU, OMG, 4SU, OMU, ZN, 0TD, UR3, 31H, 7MG, K, 5MC, 2MA, MA6, 4OC, 6IF, SF4, MIA, PSU, OMC, 2MG, 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	0.50	0/69011	0.98	74/107720 (0.1%)
1	2A	0.38	0/67295	0.86	20/105042 (0.0%)
2	1B	0.44	1/2882 (0.0%)	0.88	0/4494
2	2B	0.42	1/2879 (0.0%)	0.87	1/4487 (0.0%)
3	1D	0.35	0/2186	0.57	0/2944
3	2D	0.31	0/2186	0.51	0/2944
4	1E	0.35	0/1592	0.54	0/2149
4	2E	0.31	0/1592	0.51	0/2149
5	1F	0.33	0/1619	0.54	1/2193 (0.0%)
5	2F	0.29	0/1615	0.49	0/2188
6	1G	0.30	0/1448	0.52	0/1957
6	2G	0.30	0/1453	0.46	0/1963
7	1H	0.31	0/1356	0.49	0/1834
7	2H	0.29	0/1356	0.46	0/1834
8	1I	0.27	0/1112	0.49	0/1514
8	2I	0.27	0/1079	0.50	0/1475
9	1N	0.32	0/1144	0.50	0/1543
9	2N	0.31	0/1144	0.46	0/1543
10	1O	0.33	0/943	0.53	0/1269
10	2O	0.30	0/943	0.51	0/1269
11	1P	0.33	0/1152	0.57	0/1533
11	2P	0.30	0/1152	0.53	0/1533
12	1Q	0.35	0/1143	0.52	0/1527
12	2Q	0.30	0/1143	0.48	0/1527
13	1R	0.33	0/982	0.54	0/1312
13	2R	0.27	0/982	0.49	0/1312
14	1S	0.30	0/883	0.52	0/1176
14	2S	0.30	0/880	0.51	0/1172
15	1T	0.33	0/1105	0.52	0/1477
15	2T	0.29	0/1097	0.49	0/1468
16	1U	0.37	0/977	0.53	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.29	0/977	0.44	0/1301
17	1V	0.35	0/782	0.57	0/1049
17	2V	0.29	0/782	0.50	0/1049
18	1W	0.36	0/897	0.53	0/1205
18	2W	0.30	0/897	0.47	0/1205
19	1X	0.35	0/764	0.54	0/1025
19	2X	0.30	0/764	0.53	0/1025
20	1Y	0.33	0/819	0.53	0/1095
20	2Y	0.29	0/819	0.52	0/1095
21	1Z	0.32	0/1267	0.51	0/1717
21	2Z	0.29	0/1299	0.49	0/1763
22	10	0.35	0/662	0.54	0/881
22	20	0.32	0/662	0.50	0/881
23	11	0.32	0/762	0.50	0/1014
23	21	0.30	0/762	0.52	0/1014
24	12	0.30	0/590	0.46	0/781
24	22	0.28	0/590	0.42	0/781
25	13	0.30	0/474	0.54	0/635
25	23	0.28	0/469	0.43	0/630
26	14	0.32	0/565	0.54	0/761
26	24	0.30	0/545	0.55	1/737 (0.1%)
27	15	0.34	0/469	0.58	0/635
27	25	0.30	0/469	0.49	0/635
28	16	0.33	0/460	0.51	0/613
28	26	0.28	0/456	0.50	0/608
29	17	0.34	0/426	0.50	0/561
29	27	0.27	0/426	0.47	0/561
30	18	0.32	0/525	0.54	0/691
30	28	0.27	0/525	0.48	0/691
31	19	0.32	0/310	0.52	0/407
31	29	0.29	0/310	0.51	0/407
32	1a	0.37	0/35795	0.88	29/55864 (0.1%)
32	2a	0.36	2/35886 (0.0%)	0.90	38/56005 (0.1%)
33	1b	0.29	0/1881	0.49	0/2542
33	2b	0.31	0/1860	0.49	0/2518
34	1c	0.28	0/1572	0.46	0/2126
34	2c	0.30	0/1566	0.50	0/2119
35	1d	0.28	0/1685	0.47	0/2262
35	2d	0.28	0/1704	0.47	0/2284
36	1e	0.29	0/1145	0.51	0/1543
36	2e	0.29	0/1149	0.49	0/1548
37	1f	0.28	0/823	0.48	0/1115
37	2f	0.29	0/829	0.47	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.27	0/1250	0.44	0/1679
38	2g	0.28	0/1254	0.44	0/1683
39	1h	0.29	0/1108	0.47	0/1494
39	2h	0.27	0/1108	0.45	0/1494
40	1i	0.29	0/1002	0.51	0/1346
40	2i	0.30	0/997	0.49	0/1343
41	1j	0.27	0/722	0.48	0/982
41	2j	0.29	0/727	0.51	0/988
42	1k	0.28	0/844	0.47	0/1145
42	2k	0.27	0/848	0.47	0/1149
43	1l	0.29	0/937	0.50	0/1260
43	2l	0.29	0/937	0.47	0/1260
44	1m	0.29	0/969	0.49	0/1302
44	2m	0.29	0/961	0.49	0/1291
45	1n	0.30	0/501	0.47	0/664
45	2n	0.30	0/501	0.48	0/664
46	1o	0.27	0/739	0.43	0/985
46	2o	0.26	0/739	0.43	0/985
47	1p	0.28	0/697	0.50	0/939
47	2p	0.27	0/693	0.51	0/935
48	1q	0.29	0/836	0.47	0/1117
48	2q	0.29	0/836	0.49	0/1117
49	1r	0.28	0/560	0.51	0/746
49	2r	0.27	0/560	0.49	0/746
50	1s	0.26	0/667	0.53	0/900
50	2s	0.30	0/661	0.56	0/893
51	1t	0.27	0/730	0.44	0/965
51	2t	0.26	0/729	0.42	0/965
52	1u	0.25	0/203	0.43	0/266
52	2u	0.27	0/203	0.46	0/266
53	1v	0.42	0/310	0.93	0/480
53	2v	0.38	0/310	0.83	0/480
54	1w	0.52	1/1537 (0.1%)	1.08	6/2390 (0.3%)
54	2w	0.50	0/1487	1.09	2/2311 (0.1%)
55	1x	0.53	3/1700 (0.2%)	1.15	18/2650 (0.7%)
55	2x	0.45	0/1700	1.01	8/2650 (0.3%)
56	1y	0.51	1/1606 (0.1%)	1.07	5/2497 (0.2%)
56	2y	0.49	1/1583 (0.1%)	0.99	0/2459
All	All	0.39	10/316502 (0.0%)	0.83	203/473837 (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
51	1t	0	1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	2y	1	G	OP3-P	-10.24	1.48	1.61
54	1w	1	G	OP3-P	-10.23	1.48	1.61
2	2B	1	U	OP3-P	-10.19	1.49	1.61
2	1B	1	U	OP3-P	-10.11	1.49	1.61
56	1y	1	G	OP3-P	-10.10	1.49	1.61
32	2a	1272	G	N1-C2	-7.91	1.31	1.37
32	2a	1272	G	C6-N1	-7.19	1.34	1.39
55	1x	22	G	N7-C5	5.58	1.42	1.39
55	1x	22	G	C8-N7	5.15	1.34	1.30
55	1x	46	G	C6-N1	5.05	1.43	1.39

All (203) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1272	G	N3-C2-N2	20.12	133.99	119.90
32	2a	1263	C	N1-C2-O2	20.03	130.92	118.90
32	2a	1272	G	C5-C6-O6	16.86	138.72	128.60
32	2a	1272	G	N1-C2-N2	-16.35	101.48	116.20
32	2a	1272	G	C6-N1-C2	12.00	132.30	125.10
32	2a	1263	C	C2-N3-C4	11.38	125.59	119.90
32	2a	1263	C	N3-C2-O2	-10.96	114.23	121.90
32	2a	1263	C	C5-C6-N1	10.54	126.27	121.00
2	2B	80	U	O4'-C1'-N1	10.22	116.38	108.20
32	2a	1272	G	C5-C6-N1	-9.70	106.65	111.50
55	1x	46	G	C6-N1-C2	-9.65	119.31	125.10
1	1A	1063	G	C5-C6-O6	9.63	134.38	128.60
1	1A	1075	C	N1-C2-O2	9.08	124.35	118.90
32	1a	1030(B)	C	C2-N1-C1'	8.88	128.57	118.80
1	1A	975	C	N1-C2-O2	-8.81	113.61	118.90
32	2a	1272	G	N1-C6-O6	-8.81	114.61	119.90
55	1x	14	A	C5-N7-C8	8.72	108.26	103.90
54	1w	47	U	C2-N1-C1'	8.69	128.12	117.70
55	1x	22	G	N3-C4-N9	-8.67	120.80	126.00
1	1A	1352	U	O5'-P-OP1	-8.50	98.05	105.70
55	1x	14	A	C4-C5-C6	8.45	121.22	117.00
32	2a	1029	C	N1-C2-O2	8.41	123.95	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	801	G	O5'-P-OP2	-8.41	98.13	105.70
55	2x	46	G	C6-N1-C2	-8.38	120.07	125.10
1	1A	512	G	O4'-C1'-N9	8.29	114.83	108.20
1	1A	2167	U	C2-N1-C1'	8.12	127.44	117.70
1	2A	2136	C	N1-C2-O2	8.10	123.76	118.90
32	1a	1034	G	C6-N1-C2	8.05	129.93	125.10
1	1A	1086	A	N1-C6-N6	-7.99	113.80	118.60
55	1x	22	G	C4-C5-C6	-7.99	114.01	118.80
32	1a	1030(B)	C	N1-C2-O2	7.98	123.69	118.90
55	1x	22	G	C8-N9-C1'	7.78	137.11	127.00
32	2a	1263	C	C2-N1-C1'	7.77	127.35	118.80
1	1A	576	U	O5'-P-OP1	-7.72	98.75	105.70
55	1x	22	G	C5-N7-C8	-7.69	100.45	104.30
56	1y	33	U	C2-N1-C1'	7.57	126.79	117.70
32	1a	1030(B)	C	C6-N1-C2	-7.57	117.27	120.30
1	1A	527	C	N1-C2-O2	-7.52	114.39	118.90
32	2a	1272	G	C4-N9-C1'	7.49	136.24	126.50
1	1A	801	G	O5'-P-OP2	-7.47	98.98	105.70
1	1A	1075	C	C2-N3-C4	7.46	123.63	119.90
1	1A	588	U	O5'-P-OP2	-7.44	99.00	105.70
32	2a	1263	C	C4-C5-C6	-7.42	113.69	117.40
1	1A	2248	C	O5'-P-OP2	-7.40	99.04	105.70
1	1A	2554	U	O5'-P-OP1	-7.33	99.11	105.70
54	1w	47	U	N1-C2-O2	7.33	127.93	122.80
1	2A	2711	A	O5'-P-OP1	-7.12	99.29	105.70
32	2a	1272	G	C8-N9-C1'	-7.02	117.87	127.00
32	2a	1263	C	C6-N1-C2	-7.01	117.50	120.30
1	1A	624	C	O5'-P-OP1	-6.95	99.44	105.70
1	1A	948	G	O5'-P-OP1	-6.92	99.47	105.70
55	1x	14	A	C5-C6-N1	-6.91	114.24	117.70
1	1A	2167	U	N1-C2-O2	6.88	127.61	122.80
32	1a	1034	G	C5-C6-O6	6.87	132.72	128.60
55	2x	14	A	C5-N7-C8	6.81	107.31	103.90
32	2a	754	C	C2-N1-C1'	6.64	126.11	118.80
55	2x	14	A	C4-C5-C6	6.62	120.31	117.00
1	1A	2167	U	N3-C2-O2	-6.61	117.58	122.20
55	1x	22	G	C4-N9-C1'	-6.58	117.94	126.50
55	1x	46	G	N3-C2-N2	-6.58	115.29	119.90
32	1a	1030(B)	C	N3-C2-O2	-6.57	117.30	121.90
1	1A	2430	A	C2-N3-C4	6.56	113.88	110.60
32	1a	266	G	P-O3'-C3'	6.54	127.55	119.70
32	2a	1029	C	N3-C2-O2	-6.54	117.32	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1063	G	N3-C2-N2	6.51	124.46	119.90
1	1A	2129	C	N1-C2-O2	6.49	122.80	118.90
1	1A	787	U	O5'-P-OP1	-6.49	99.86	105.70
55	1x	22	G	N3-C4-C5	6.49	131.84	128.60
55	1x	22	G	C6-C5-N7	6.47	134.28	130.40
1	1A	226	G	O4'-C1'-N9	6.45	113.36	108.20
1	1A	975	C	C2-N1-C1'	-6.44	111.72	118.80
1	1A	847	U	C2-N1-C1'	6.42	125.40	117.70
55	1x	22	G	N1-C6-O6	-6.41	116.05	119.90
55	2x	22	G	C5-N7-C8	-6.37	101.12	104.30
32	1a	1025	U	N1-C2-O2	6.35	127.25	122.80
1	1A	567	A	O5'-P-OP1	-6.32	100.01	105.70
1	1A	1342	A	O5'-P-OP2	-6.32	100.01	105.70
1	2A	1313	U	C2-N1-C1'	6.31	125.27	117.70
32	2a	1263	C	N1-C2-N3	-6.26	114.82	119.20
54	1w	47	U	N3-C2-O2	-6.25	117.82	122.20
1	1A	1992	G	P-O3'-C3'	6.25	127.20	119.70
32	2a	1272	G	C2-N3-C4	-6.25	108.78	111.90
1	1A	1063	G	C6-N1-C2	6.24	128.85	125.10
32	2a	266	G	N3-C4-C5	-6.19	125.50	128.60
1	1A	1080	C	N1-C2-O2	6.18	122.61	118.90
1	1A	1776	G	O5'-P-OP2	-6.14	100.17	105.70
32	2a	79	G	C5-C6-O6	6.10	132.26	128.60
1	1A	996	A	O5'-P-OP1	-6.06	100.25	105.70
1	1A	2629	A	P-O3'-C3'	6.04	126.95	119.70
32	1a	1002	G	C4-N9-C1'	6.04	134.36	126.50
32	2a	1279	A	OP1-P-O3'	6.01	118.42	105.20
32	1a	1067	A	P-O3'-C3'	6.00	126.91	119.70
32	1a	1002	G	N3-C4-N9	6.00	129.60	126.00
1	2A	752	A	P-O3'-C3'	5.98	126.88	119.70
1	1A	1075	C	C5-C4-N4	5.97	124.38	120.20
32	2a	754	C	N1-C2-O2	5.95	122.47	118.90
1	1A	2593	U	N3-C4-O4	-5.91	115.27	119.40
32	1a	841	U	C5-C6-N1	5.89	125.65	122.70
56	1y	33	U	N1-C2-O2	5.89	126.92	122.80
1	2A	1698	A	O4'-C1'-N9	5.86	112.88	108.20
1	1A	392	C	O5'-P-OP1	-5.84	100.44	105.70
32	1a	1030(B)	C	C5-C6-N1	5.84	123.92	121.00
1	2A	2155	G	C6-N1-C2	5.82	128.59	125.10
32	1a	1036	G	N3-C2-N2	-5.81	115.83	119.90
1	1A	1063	G	N1-C6-O6	-5.80	116.42	119.90
54	1w	47	U	C6-N1-C1'	-5.80	113.09	121.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	195	A	P-O3'-C3'	5.78	126.64	119.70
1	1A	845	G	O4'-C1'-N9	5.78	112.82	108.20
32	1a	1027	C	C6-N1-C1'	5.77	127.73	120.80
1	1A	250	G	C8-N9-C4	-5.75	104.10	106.40
1	1A	1075	C	N3-C2-O2	-5.74	117.88	121.90
55	1x	14	A	C4-C5-N7	-5.74	107.83	110.70
1	2A	1992	G	P-O3'-C3'	5.73	126.57	119.70
32	1a	1027	C	C2-N1-C1'	-5.69	112.54	118.80
1	1A	2581	G	O4'-C1'-N9	5.68	112.75	108.20
55	1x	46	G	C5-C6-N1	5.65	114.33	111.50
1	2A	1780	A	O5'-P-OP1	-5.64	100.63	105.70
32	2a	841	U	C5-C6-N1	5.63	125.52	122.70
32	1a	1030(B)	C	C6-N1-C1'	-5.63	114.05	120.80
1	2A	845	G	C4-N9-C1'	5.62	133.81	126.50
55	1x	46	G	C5-C6-O6	-5.60	125.24	128.60
1	1A	589	C	C6-N1-C2	-5.53	118.09	120.30
32	2a	1065	U	P-O3'-C3'	5.52	126.33	119.70
1	1A	2848	G	O4'-C1'-N9	5.52	112.61	108.20
32	2a	1037	C	C6-N1-C2	-5.51	118.10	120.30
1	1A	383	U	O4'-C1'-N1	5.51	112.61	108.20
1	1A	2167	U	C5-C6-N1	5.49	125.44	122.70
32	1a	1002	G	C8-N9-C1'	-5.49	119.86	127.00
1	2A	512	G	O4'-C1'-N9	5.49	112.59	108.20
1	2A	1022	G	N3-C4-N9	-5.48	122.71	126.00
1	1A	372	G	O4'-C1'-N9	5.46	112.57	108.20
1	1A	1174	A	P-O3'-C3'	5.45	126.24	119.70
32	1a	90	U	N3-C2-O2	-5.45	118.39	122.20
55	2x	46	G	C5-C6-N1	5.44	114.22	111.50
32	2a	1279	A	P-O3'-C3'	5.43	126.22	119.70
1	1A	180	G	C5-C6-O6	-5.42	125.35	128.60
32	1a	1020	U	N1-C2-O2	5.42	126.59	122.80
32	1a	754	C	N1-C2-O2	5.42	122.15	118.90
1	1A	975	C	C6-N1-C1'	5.41	127.30	120.80
32	2a	687	A	P-O3'-C3'	5.41	126.19	119.70
55	1x	14	A	C8-N9-C1'	-5.38	118.02	127.70
1	1A	793	A	O5'-P-OP2	-5.37	100.87	105.70
32	2a	65	U	P-O3'-C3'	5.36	126.13	119.70
5	1F	12	LEU	CA-CB-CG	5.35	127.61	115.30
1	1A	139(A)	G	C8-N9-C1'	-5.35	120.05	127.00
1	1A	1176	G	OP1-P-O3'	5.34	116.95	105.20
56	1y	58	A	OP1-P-O3'	5.34	116.95	105.20
1	1A	784	A	P-O3'-C3'	5.34	126.11	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2319	G	O4'-C1'-N9	5.34	112.47	108.20
1	2A	383	U	O4'-C1'-N1	5.34	112.47	108.20
32	2a	1391	U	N1-C2-O2	5.33	126.53	122.80
32	2a	266	G	P-O3'-C3'	5.33	126.09	119.70
1	1A	846	C	C6-N1-C2	5.32	122.43	120.30
56	1y	58	A	P-O3'-C3'	5.32	126.09	119.70
1	1A	881	G	N7-C8-N9	5.32	115.76	113.10
55	2x	22	G	C4-C5-C6	-5.32	115.61	118.80
1	1A	671	C	C5-C4-N4	5.31	123.92	120.20
55	1x	14	A	C4-N9-C1'	5.30	135.85	126.30
55	2x	14	A	C5-C6-N1	-5.30	115.05	117.70
32	1a	353	A	OP2-P-O3'	5.29	116.84	105.20
1	2A	576	U	O5'-P-OP1	-5.29	100.94	105.70
32	1a	1002	G	N3-C4-C5	-5.29	125.96	128.60
54	2w	13	C	OP1-P-O3'	5.26	116.78	105.20
1	2A	2136	C	N3-C2-O2	-5.26	118.22	121.90
1	1A	2873	A	O4'-C1'-N9	5.25	112.40	108.20
32	2a	1054	C	C2-N1-C1'	5.24	124.56	118.80
32	1a	754	C	C2-N1-C1'	5.24	124.56	118.80
56	1y	33	U	C6-N1-C1'	-5.23	113.87	121.20
1	1A	1080	C	C2-N3-C4	5.23	122.52	119.90
1	2A	2139	C	C2-N1-C1'	5.21	124.54	118.80
1	1A	120	U	O5'-P-OP1	-5.20	101.02	105.70
32	2a	913	A	P-O3'-C3'	5.19	125.93	119.70
32	2a	841	U	C2-N1-C1'	5.19	123.92	117.70
1	1A	1131	G	O4'-C1'-N9	5.18	112.34	108.20
1	1A	1174	A	OP1-P-O3'	5.18	116.59	105.20
32	1a	1201	A	P-O3'-C3'	5.17	125.90	119.70
54	1w	60	U	N3-C2-O2	-5.16	118.59	122.20
1	1A	975(A)	G	O5'-P-OP2	-5.14	101.07	105.70
1	1A	2609	U	C2-N1-C1'	-5.14	111.53	117.70
32	1a	1030	C	C2-N3-C4	5.14	122.47	119.90
1	1A	1253	A	N7-C8-N9	-5.13	111.23	113.80
1	1A	1177	A	O5'-P-OP1	-5.13	101.08	105.70
54	2w	13	C	P-O3'-C3'	5.13	125.86	119.70
1	1A	2005	A	OP1-P-O3'	5.12	116.46	105.20
32	1a	1531	A	N7-C8-N9	5.11	116.36	113.80
1	1A	2790	A	C2-N3-C4	5.09	113.14	110.60
1	1A	2032	G	C5-N7-C8	5.08	106.84	104.30
32	2a	1272	G	N3-C4-N9	5.08	129.05	126.00
26	24	5	ILE	C-N-CA	5.07	134.38	121.70
1	2A	845	G	C8-N9-C1'	-5.07	120.41	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	687	A	P-O3'-C3'	5.06	125.77	119.70
32	1a	90	U	N1-C2-O2	5.05	126.34	122.80
1	1A	2685	G	N1-C6-O6	-5.04	116.88	119.90
32	2a	1025	U	N1-C2-O2	5.04	126.33	122.80
1	1A	1009	A	N1-C6-N6	5.03	121.62	118.60
1	1A	746	A	O4'-C1'-N9	5.03	112.22	108.20
1	2A	265	A	O4'-C1'-N9	5.03	112.22	108.20
1	2A	2689	U	P-O3'-C3'	5.01	125.72	119.70
55	2x	22	G	C8-N9-C1'	5.01	133.52	127.00
1	1A	2714	G	O5'-P-OP2	-5.01	101.19	105.70
32	2a	754	C	C6-N1-C1'	-5.01	114.79	120.80
54	1w	47	U	C5-C6-N1	5.00	125.20	122.70
1	2A	228	A	P-O3'-C3'	5.00	125.70	119.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
51	1t	99	LEU	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	258 (94%)	14 (5%)	1 (0%)	34	54
3	2D	273/276 (99%)	253 (93%)	20 (7%)	0	100	100
4	1E	202/206 (98%)	194 (96%)	7 (4%)	1 (0%)	29	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	2E	202/206 (98%)	186 (92%)	15 (7%)	1 (0%)	29	48
5	1F	201/210 (96%)	195 (97%)	5 (2%)	1 (0%)	29	48
5	2F	201/210 (96%)	187 (93%)	12 (6%)	2 (1%)	15	28
6	1G	179/182 (98%)	166 (93%)	12 (7%)	1 (1%)	25	43
6	2G	179/182 (98%)	154 (86%)	22 (12%)	3 (2%)	9	16
7	1H	172/180 (96%)	162 (94%)	10 (6%)	0	100	100
7	2H	172/180 (96%)	156 (91%)	15 (9%)	1 (1%)	25	43
8	1I	144/148 (97%)	132 (92%)	12 (8%)	0	100	100
8	2I	144/148 (97%)	123 (85%)	19 (13%)	2 (1%)	11	20
9	1N	138/140 (99%)	131 (95%)	7 (5%)	0	100	100
9	2N	138/140 (99%)	129 (94%)	8 (6%)	1 (1%)	22	39
10	1O	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
10	2O	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
11	1P	147/150 (98%)	135 (92%)	9 (6%)	3 (2%)	7	12
11	2P	147/150 (98%)	127 (86%)	15 (10%)	5 (3%)	3	5
12	1Q	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
12	2Q	139/141 (99%)	126 (91%)	13 (9%)	0	100	100
13	1R	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
13	2R	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
14	1S	108/112 (96%)	103 (95%)	5 (5%)	0	100	100
14	2S	108/112 (96%)	96 (89%)	8 (7%)	4 (4%)	3	4
15	1T	129/146 (88%)	121 (94%)	7 (5%)	1 (1%)	19	35
15	2T	129/146 (88%)	123 (95%)	6 (5%)	0	100	100
16	1U	114/118 (97%)	114 (100%)	0	0	100	100
16	2U	114/118 (97%)	110 (96%)	4 (4%)	0	100	100
17	1V	99/101 (98%)	93 (94%)	5 (5%)	1 (1%)	15	28
17	2V	99/101 (98%)	92 (93%)	6 (6%)	1 (1%)	15	28
18	1W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
18	2W	110/113 (97%)	107 (97%)	3 (3%)	0	100	100
19	1X	93/96 (97%)	88 (95%)	3 (3%)	2 (2%)	6	10
19	2X	93/96 (97%)	88 (95%)	4 (4%)	1 (1%)	14	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	1Y	105/110 (96%)	97 (92%)	7 (7%)	1 (1%)	15	28
20	2Y	105/110 (96%)	99 (94%)	3 (3%)	3 (3%)	4	6
21	1Z	148/206 (72%)	125 (84%)	21 (14%)	2 (1%)	11	20
21	2Z	156/206 (76%)	122 (78%)	33 (21%)	1 (1%)	25	43
22	10	81/85 (95%)	78 (96%)	3 (4%)	0	100	100
22	20	81/85 (95%)	73 (90%)	7 (9%)	1 (1%)	13	24
23	11	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	14	26
23	21	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	14	26
24	12	68/72 (94%)	68 (100%)	0	0	100	100
24	22	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
25	13	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
25	23	57/60 (95%)	52 (91%)	4 (7%)	1 (2%)	8	14
26	14	67/71 (94%)	54 (81%)	8 (12%)	5 (8%)	1	1
26	24	67/71 (94%)	47 (70%)	17 (25%)	3 (4%)	2	3
27	15	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	25	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
28	16	51/54 (94%)	51 (100%)	0	0	100	100
28	26	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
29	17	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
29	27	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
30	18	62/65 (95%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	33 (94%)	1 (3%)	1 (3%)	4	6
33	1b	229/256 (90%)	190 (83%)	31 (14%)	8 (4%)	3	4
33	2b	229/256 (90%)	180 (79%)	40 (18%)	9 (4%)	3	4
34	1c	204/239 (85%)	180 (88%)	23 (11%)	1 (0%)	29	48
34	2c	204/239 (85%)	169 (83%)	31 (15%)	4 (2%)	7	12
35	1d	206/209 (99%)	187 (91%)	18 (9%)	1 (0%)	29	48
35	2d	206/209 (99%)	187 (91%)	17 (8%)	2 (1%)	15	28
36	1e	146/162 (90%)	133 (91%)	12 (8%)	1 (1%)	22	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	2e	146/162 (90%)	125 (86%)	17 (12%)	4 (3%)	5	7
37	1f	98/101 (97%)	91 (93%)	7 (7%)	0	100	100
37	2f	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
38	1g	153/156 (98%)	139 (91%)	12 (8%)	2 (1%)	12	21
38	2g	153/156 (98%)	135 (88%)	16 (10%)	2 (1%)	12	21
39	1h	135/138 (98%)	126 (93%)	9 (7%)	0	100	100
39	2h	135/138 (98%)	122 (90%)	12 (9%)	1 (1%)	22	39
40	1i	125/128 (98%)	112 (90%)	12 (10%)	1 (1%)	19	35
40	2i	125/128 (98%)	101 (81%)	23 (18%)	1 (1%)	19	35
41	1j	95/105 (90%)	81 (85%)	11 (12%)	3 (3%)	4	5
41	2j	94/105 (90%)	76 (81%)	14 (15%)	4 (4%)	2	3
42	1k	112/129 (87%)	99 (88%)	10 (9%)	3 (3%)	5	7
42	2k	112/129 (87%)	100 (89%)	10 (9%)	2 (2%)	8	14
43	1l	119/132 (90%)	111 (93%)	8 (7%)	0	100	100
43	2l	119/132 (90%)	110 (92%)	8 (7%)	1 (1%)	19	35
44	1m	121/126 (96%)	109 (90%)	10 (8%)	2 (2%)	9	16
44	2m	120/126 (95%)	97 (81%)	21 (18%)	2 (2%)	9	16
45	1n	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
45	2n	58/61 (95%)	51 (88%)	6 (10%)	1 (2%)	9	16
46	1o	86/89 (97%)	81 (94%)	3 (4%)	2 (2%)	6	10
46	2o	86/89 (97%)	79 (92%)	6 (7%)	1 (1%)	13	24
47	1p	80/88 (91%)	73 (91%)	6 (8%)	1 (1%)	12	21
47	2p	80/88 (91%)	71 (89%)	9 (11%)	0	100	100
48	1q	97/105 (92%)	92 (95%)	5 (5%)	0	100	100
48	2q	97/105 (92%)	86 (89%)	10 (10%)	1 (1%)	15	28
49	1r	66/88 (75%)	62 (94%)	4 (6%)	0	100	100
49	2r	66/88 (75%)	61 (92%)	5 (8%)	0	100	100
50	1s	81/93 (87%)	71 (88%)	8 (10%)	2 (2%)	5	8
50	2s	81/93 (87%)	64 (79%)	15 (18%)	2 (2%)	5	8
51	1t	94/106 (89%)	85 (90%)	6 (6%)	3 (3%)	4	5
51	2t	94/106 (89%)	87 (93%)	3 (3%)	4 (4%)	2	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	1u	21/27 (78%)	21 (100%)	0	0	100	100
52	2u	21/27 (78%)	13 (62%)	8 (38%)	0	100	100
All	All	11370/12128 (94%)	10356 (91%)	891 (8%)	123 (1%)	14	26

All (123) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
11	1P	38	GLN
21	1Z	52	SER
21	1Z	163	LEU
23	11	3	LYS
26	14	47	GLN
33	1b	22	LYS
33	1b	126	GLU
38	1g	80	VAL
44	1m	67	GLU
50	1s	81	ARG
6	2G	51	ARG
8	2I	10	GLU
11	2P	36	LYS
20	2Y	55	TYR
33	2b	17	PHE
33	2b	123	ALA
38	2g	80	VAL
50	2s	81	ARG
11	1P	36	LYS
17	1V	79	VAL
19	1X	93	GLU
26	14	57	GLU
26	14	62	ARG
33	1b	17	PHE
36	1e	85	GLY
41	1j	79	ARG
42	1k	49	GLY
42	1k	77	MET
46	1o	88	ARG
5	2F	130	ALA
6	2G	42	GLY
11	2P	29	LYS
11	2P	44	GLY

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Mol	Chain	Res	Type
14	2S	96	GLY
17	2V	79	VAL
19	2X	94	GLY
21	2Z	146	ILE
23	2I	3	LYS
33	2b	74	LYS
36	2e	77	PRO
38	2g	55	GLY
41	2j	79	ARG
42	2k	49	GLY
46	2o	88	ARG
48	2q	68	ARG
50	2s	12	ASP
4	1E	52	LEU
20	1Y	54	LYS
26	14	49	PHE
33	1b	8	LYS
41	1j	29	ARG
50	1s	29	ARG
51	1t	47	GLY
4	2E	52	LEU
6	2G	47	LYS
7	2H	47	GLU
8	2I	39	ALA
11	2P	45	LEU
14	2S	20	ARG
14	2S	84	GLN
20	2Y	54	LYS
22	20	73	GLY
26	24	49	PHE
33	2b	9	GLU
33	2b	16	HIS
33	2b	20	GLU
34	2c	111	LEU
35	2d	164	ALA
39	2h	68	ARG
42	2k	105	VAL
43	2l	105	TYR
3	1D	262	ARG
15	1T	37	GLY
33	1b	155	LEU
38	1g	52	GLU

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Mol	Chain	Res	Type
40	1i	54	ASP
41	1j	78	ASN
46	1o	87	ILE
47	1p	76	GLN
51	1t	96	GLY
5	2F	146	ALA
11	2P	38	GLN
26	24	11	PRO
26	24	39	CYS
33	2b	106	LYS
33	2b	126	GLU
34	2c	53	ALA
34	2c	91	LEU
44	2m	87	TYR
45	2n	14	PRO
51	2t	10	LEU
51	2t	98	PRO
6	1G	43	LEU
11	1P	29	LYS
19	1X	2	LYS
26	14	53	GLU
33	1b	124	SER
33	1b	129	GLU
33	1b	231	GLU
34	1c	107	GLN
35	1d	88	VAL
51	1t	100	ILE
9	2N	8	GLN
14	2S	32	LEU
34	2c	156	ARG
36	2e	85	GLY
40	2i	56	LEU
41	2j	75	ILE
44	2m	106	ASN
51	2t	99	LEU
25	23	59	VAL
33	2b	231	GLU
36	2e	96	PRO
41	2j	41	PRO
44	1m	4	ILE
42	1k	105	VAL
35	2d	136	PRO

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Mol	Chain	Res	Type
41	2j	50	ILE
31	29	21	GLY
36	2e	69	VAL
51	2t	47	GLY
20	2Y	27	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	215/218 (99%)	201 (94%)	14 (6%)	17	33
3	2D	215/218 (99%)	205 (95%)	10 (5%)	26	49
4	1E	164/166 (99%)	151 (92%)	13 (8%)	12	24
4	2E	164/166 (99%)	155 (94%)	9 (6%)	21	41
5	1F	160/166 (96%)	149 (93%)	11 (7%)	15	30
5	2F	159/166 (96%)	152 (96%)	7 (4%)	28	52
6	1G	143/156 (92%)	129 (90%)	14 (10%)	8	15
6	2G	143/156 (92%)	123 (86%)	20 (14%)	3	6
7	1H	144/148 (97%)	137 (95%)	7 (5%)	25	47
7	2H	144/148 (97%)	130 (90%)	14 (10%)	8	16
8	1I	113/124 (91%)	95 (84%)	18 (16%)	2	4
8	2I	105/124 (85%)	94 (90%)	11 (10%)	7	13
9	1N	118/119 (99%)	111 (94%)	7 (6%)	19	37
9	2N	118/119 (99%)	110 (93%)	8 (7%)	16	30
10	1O	100/100 (100%)	97 (97%)	3 (3%)	41	68
10	2O	100/100 (100%)	96 (96%)	4 (4%)	31	56
11	1P	115/116 (99%)	107 (93%)	8 (7%)	15	29
11	2P	115/116 (99%)	108 (94%)	7 (6%)	18	36
12	1Q	111/111 (100%)	105 (95%)	6 (5%)	22	42
12	2Q	111/111 (100%)	104 (94%)	7 (6%)	18	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	1R	101/101 (100%)	98 (97%)	3 (3%)	41	68
13	2R	101/101 (100%)	97 (96%)	4 (4%)	31	56
14	1S	86/88 (98%)	78 (91%)	8 (9%)	9	17
14	2S	85/88 (97%)	72 (85%)	13 (15%)	2	5
15	1T	115/127 (91%)	110 (96%)	5 (4%)	29	53
15	2T	113/127 (89%)	106 (94%)	7 (6%)	18	35
16	1U	93/94 (99%)	85 (91%)	8 (9%)	10	20
16	2U	93/94 (99%)	87 (94%)	6 (6%)	17	33
17	1V	80/82 (98%)	77 (96%)	3 (4%)	33	58
17	2V	80/82 (98%)	70 (88%)	10 (12%)	4	8
18	1W	90/92 (98%)	86 (96%)	4 (4%)	28	52
18	2W	90/92 (98%)	87 (97%)	3 (3%)	38	64
19	1X	77/78 (99%)	75 (97%)	2 (3%)	46	72
19	2X	77/78 (99%)	73 (95%)	4 (5%)	23	44
20	1Y	85/91 (93%)	81 (95%)	4 (5%)	26	49
20	2Y	85/91 (93%)	76 (89%)	9 (11%)	6	13
21	1Z	135/179 (75%)	125 (93%)	10 (7%)	13	27
21	2Z	137/179 (76%)	122 (89%)	15 (11%)	6	12
22	10	65/67 (97%)	63 (97%)	2 (3%)	40	67
22	20	65/67 (97%)	62 (95%)	3 (5%)	27	50
23	11	80/83 (96%)	79 (99%)	1 (1%)	69	87
23	21	80/83 (96%)	77 (96%)	3 (4%)	33	58
24	12	65/67 (97%)	61 (94%)	4 (6%)	18	35
24	22	65/67 (97%)	59 (91%)	6 (9%)	9	18
25	13	51/52 (98%)	47 (92%)	4 (8%)	12	24
25	23	50/52 (96%)	48 (96%)	2 (4%)	31	56
26	14	59/63 (94%)	51 (86%)	8 (14%)	3	7
26	24	53/63 (84%)	42 (79%)	11 (21%)	1	2
27	15	50/52 (96%)	48 (96%)	2 (4%)	31	56
27	25	50/52 (96%)	47 (94%)	3 (6%)	19	37
28	16	51/52 (98%)	47 (92%)	4 (8%)	12	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	26	50/52 (96%)	47 (94%)	3 (6%)	19	37
29	17	41/42 (98%)	36 (88%)	5 (12%)	5	9
29	27	41/42 (98%)	37 (90%)	4 (10%)	8	15
30	18	54/55 (98%)	50 (93%)	4 (7%)	13	27
30	28	54/55 (98%)	49 (91%)	5 (9%)	9	17
31	19	34/34 (100%)	33 (97%)	1 (3%)	42	69
31	29	34/34 (100%)	33 (97%)	1 (3%)	42	69
33	1b	192/220 (87%)	166 (86%)	26 (14%)	4	7
33	2b	187/220 (85%)	162 (87%)	25 (13%)	4	7
34	1c	142/188 (76%)	128 (90%)	14 (10%)	8	15
34	2c	140/188 (74%)	124 (89%)	16 (11%)	5	11
35	1d	169/181 (93%)	153 (90%)	16 (10%)	8	17
35	2d	173/181 (96%)	159 (92%)	14 (8%)	11	23
36	1e	113/123 (92%)	103 (91%)	10 (9%)	10	19
36	2e	114/123 (93%)	102 (90%)	12 (10%)	7	13
37	1f	84/90 (93%)	80 (95%)	4 (5%)	25	48
37	2f	85/90 (94%)	79 (93%)	6 (7%)	14	28
38	1g	119/127 (94%)	110 (92%)	9 (8%)	13	25
38	2g	120/127 (94%)	104 (87%)	16 (13%)	4	7
39	1h	114/119 (96%)	108 (95%)	6 (5%)	22	43
39	2h	114/119 (96%)	102 (90%)	12 (10%)	7	13
40	1i	90/99 (91%)	79 (88%)	11 (12%)	5	9
40	2i	89/99 (90%)	78 (88%)	11 (12%)	4	9
41	1j	66/92 (72%)	60 (91%)	6 (9%)	9	18
41	2j	69/92 (75%)	61 (88%)	8 (12%)	5	10
42	1k	82/99 (83%)	75 (92%)	7 (8%)	10	21
42	2k	83/99 (84%)	74 (89%)	9 (11%)	6	12
43	1l	96/108 (89%)	92 (96%)	4 (4%)	30	54
43	2l	96/108 (89%)	88 (92%)	8 (8%)	11	22
44	1m	93/101 (92%)	84 (90%)	9 (10%)	8	16
44	2m	92/101 (91%)	82 (89%)	10 (11%)	6	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	1n	49/50 (98%)	47 (96%)	2 (4%)	30	55
45	2n	49/50 (98%)	44 (90%)	5 (10%)	7	14
46	1o	78/80 (98%)	76 (97%)	2 (3%)	46	72
46	2o	78/80 (98%)	71 (91%)	7 (9%)	9	19
47	1p	69/74 (93%)	61 (88%)	8 (12%)	5	10
47	2p	68/74 (92%)	63 (93%)	5 (7%)	13	27
48	1q	94/97 (97%)	92 (98%)	2 (2%)	53	78
48	2q	94/97 (97%)	87 (93%)	7 (7%)	13	27
49	1r	59/77 (77%)	57 (97%)	2 (3%)	37	63
49	2r	59/77 (77%)	55 (93%)	4 (7%)	16	30
50	1s	69/80 (86%)	66 (96%)	3 (4%)	29	53
50	2s	67/80 (84%)	58 (87%)	9 (13%)	4	7
51	1t	70/82 (85%)	66 (94%)	4 (6%)	20	39
51	2t	70/82 (85%)	66 (94%)	4 (6%)	20	39
52	1u	18/22 (82%)	18 (100%)	0	100	100
52	2u	18/22 (82%)	16 (89%)	2 (11%)	6	11
All	All	9303/10064 (92%)	8576 (92%)	727 (8%)	12	24

All (727) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	32	SER
3	1D	88	ARG
3	1D	106	ILE
3	1D	113	VAL
3	1D	122	ASP
3	1D	155	LEU
3	1D	162	SER
3	1D	211	ARG
3	1D	221	VAL
3	1D	229	VAL
3	1D	242	ARG
3	1D	259	THR
3	1D	260	ARG
3	1D	273	ARG
4	1E	1	MET

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Mol	Chain	Res	Type
4	1E	12	THR
4	1E	41	LYS
4	1E	45	THR
4	1E	47	VAL
4	1E	73	GLU
4	1E	83	ASP
4	1E	93	VAL
4	1E	113	PHE
4	1E	116	VAL
4	1E	181	LEU
4	1E	184	VAL
4	1E	195	LEU
5	1F	24	LEU
5	1F	27	GLU
5	1F	32	LEU
5	1F	53	THR
5	1F	70	THR
5	1F	74	ARG
5	1F	132	VAL
5	1F	140	LEU
5	1F	144	LYS
5	1F	168	ARG
5	1F	192	LEU
6	1G	3	LEU
6	1G	5	VAL
6	1G	7	LEU
6	1G	21	ARG
6	1G	31	VAL
6	1G	43	LEU
6	1G	82	LEU
6	1G	109	VAL
6	1G	126	ASP
6	1G	133	LEU
6	1G	139	LEU
6	1G	140	ILE
6	1G	149	VAL
6	1G	159	VAL
7	1H	33	LEU
7	1H	45	VAL
7	1H	49	VAL
7	1H	76	VAL
7	1H	95	ARG

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Mol	Chain	Res	Type
7	1H	119	GLU
7	1H	127	GLU
8	1I	5	LEU
8	1I	10	GLU
8	1I	38	LEU
8	1I	40	THR
8	1I	41	GLU
8	1I	44	LEU
8	1I	47	LEU
8	1I	68	LEU
8	1I	85	GLU
8	1I	92	VAL
8	1I	95	LYS
8	1I	101	LEU
8	1I	108	THR
8	1I	116	LEU
8	1I	117	GLU
8	1I	133	HIS
8	1I	140	LEU
8	1I	142	VAL
9	1N	1	MET
9	1N	5	VAL
9	1N	14	VAL
9	1N	28	THR
9	1N	48	MET
9	1N	61	ARG
9	1N	67	LEU
10	1O	28	SER
10	1O	52	VAL
10	1O	89	ASN
11	1P	1	MET
11	1P	7	ARG
11	1P	15	ARG
11	1P	45	LEU
11	1P	76	LYS
11	1P	119	GLU
11	1P	125	VAL
11	1P	148	LEU
12	1Q	7	MET
12	1Q	16	ARG
12	1Q	75	THR
12	1Q	109	VAL

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Mol	Chain	Res	Type
12	1Q	127	ILE
12	1Q	133	ARG
13	1R	36	THR
13	1R	67	LEU
13	1R	114	VAL
14	1S	14	VAL
14	1S	15	ARG
14	1S	36	TYR
14	1S	49	VAL
14	1S	50	SER
14	1S	68	GLN
14	1S	85	VAL
14	1S	110	LEU
15	1T	28	VAL
15	1T	49	VAL
15	1T	96	ARG
15	1T	108	ARG
15	1T	125	ARG
16	1U	8	VAL
16	1U	31	SER
16	1U	74	LEU
16	1U	84	LYS
16	1U	85	LYS
16	1U	95	LEU
16	1U	100	VAL
16	1U	111	GLU
17	1V	6	LYS
17	1V	79	VAL
17	1V	100	ARG
18	1W	11	ARG
18	1W	15	ARG
18	1W	17	VAL
18	1W	96	ILE
19	1X	35	THR
19	1X	70	LEU
20	1Y	61	ILE
20	1Y	91	GLU
20	1Y	99	CYS
20	1Y	106	LEU
21	1Z	18	LEU
21	1Z	49	ARG
21	1Z	104	PHE

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Mol	Chain	Res	Type
21	1Z	128	VAL
21	1Z	129	SER
21	1Z	136	PHE
21	1Z	139	VAL
21	1Z	154	ASP
21	1Z	155	LEU
21	1Z	170	THR
22	10	7	LEU
22	10	10	THR
23	11	35	THR
24	12	3	LEU
24	12	4	SER
24	12	19	VAL
24	12	40	SER
25	13	23	LEU
25	13	35	ARG
25	13	54	VAL
25	13	55	ARG
26	14	47	GLN
26	14	49	PHE
26	14	52	THR
26	14	53	GLU
26	14	59	PHE
26	14	60	GLN
26	14	63	TYR
26	14	67	TYR
27	15	40	LYS
27	15	55	ARG
28	16	19	ARG
28	16	24	GLU
28	16	44	ARG
28	16	47	THR
29	17	24	THR
29	17	32	LYS
29	17	41	ARG
29	17	43	THR
29	17	46	VAL
30	18	14	VAL
30	18	31	HIS
30	18	34	TRP
30	18	52	LYS
31	19	18	ARG

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Mol	Chain	Res	Type
33	1b	8	LYS
33	1b	12	GLU
33	1b	17	PHE
33	1b	24	TRP
33	1b	35	GLU
33	1b	54	THR
33	1b	64	ARG
33	1b	76	GLN
33	1b	80	ILE
33	1b	82	ARG
33	1b	95	GLN
33	1b	104	ASN
33	1b	127	ILE
33	1b	133	LYS
33	1b	160	ASP
33	1b	163	PHE
33	1b	185	ILE
33	1b	192	SER
33	1b	196	LEU
33	1b	208	ILE
33	1b	212	GLN
33	1b	215	LEU
33	1b	221	LEU
33	1b	223	ILE
33	1b	233	SER
33	1b	236	TYR
34	1c	3	ASN
34	1c	8	ILE
34	1c	20	SER
34	1c	28	GLN
34	1c	68	VAL
34	1c	82	GLU
34	1c	89	GLU
34	1c	91	LEU
34	1c	98	ASN
34	1c	131	ARG
34	1c	178	LEU
34	1c	190	ARG
34	1c	195	VAL
34	1c	201	TYR
35	1d	3	ARG
35	1d	5	ILE

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Mol	Chain	Res	Type
35	1d	10	ARG
35	1d	19	LEU
35	1d	49	ARG
35	1d	77	ASN
35	1d	88	VAL
35	1d	135	LEU
35	1d	140	VAL
35	1d	144	ASP
35	1d	158	ILE
35	1d	177	ASP
35	1d	188	LEU
35	1d	193	ASP
35	1d	194	LEU
35	1d	200	GLU
36	1e	10	MET
36	1e	12	LEU
36	1e	20	GLN
36	1e	41	VAL
36	1e	51	VAL
36	1e	53	LEU
36	1e	56	GLN
36	1e	63	ARG
36	1e	67	VAL
36	1e	116	THR
37	1f	36	ARG
37	1f	55	ASP
37	1f	72	VAL
37	1f	75	LEU
38	1g	3	ARG
38	1g	12	LEU
38	1g	31	MET
38	1g	50	ILE
38	1g	79	ARG
38	1g	104	LEU
38	1g	110	GLN
38	1g	113	GLU
38	1g	115	ARG
39	1h	23	SER
39	1h	29	SER
39	1h	52	ASP
39	1h	54	ASP
39	1h	112	LEU

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Mol	Chain	Res	Type
39	1h	133	LEU
40	1i	7	THR
40	1i	23	ASN
40	1i	41	VAL
40	1i	50	LEU
40	1i	64	THR
40	1i	88	TYR
40	1i	96	LEU
40	1i	97	LYS
40	1i	103	THR
40	1i	121	ARG
40	1i	128	ARG
41	1j	51	ARG
41	1j	55	LYS
41	1j	81	THR
41	1j	92	THR
41	1j	95	GLU
41	1j	98	ILE
42	1k	25	TYR
42	1k	31	THR
42	1k	48	ILE
42	1k	87	THR
42	1k	107	SER
42	1k	109	VAL
42	1k	114	VAL
43	1l	18	VAL
43	1l	40	VAL
43	1l	54	LYS
43	1l	83	VAL
44	1m	4	ILE
44	1m	14	ARG
44	1m	19	LEU
44	1m	32	GLU
44	1m	43	THR
44	1m	49	THR
44	1m	64	TRP
44	1m	70	LEU
44	1m	94	ARG
45	1n	18	VAL
45	1n	60	SER
46	1o	39	LEU
46	1o	76	GLU

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Mol	Chain	Res	Type
47	1p	19	ILE
47	1p	20	VAL
47	1p	21	VAL
47	1p	27	LYS
47	1p	45	THR
47	1p	50	LYS
47	1p	62	VAL
47	1p	72	ARG
48	1q	9	VAL
48	1q	57	VAL
49	1r	63	GLN
49	1r	82	THR
50	1s	6	LYS
50	1s	32	LYS
50	1s	35	SER
51	1t	10	LEU
51	1t	13	LEU
51	1t	24	LEU
51	1t	84	LEU
3	2D	3	VAL
3	2D	88	ARG
3	2D	106	ILE
3	2D	113	VAL
3	2D	173	VAL
3	2D	221	VAL
3	2D	229	VAL
3	2D	242	ARG
3	2D	259	THR
3	2D	275	LYS
4	2E	1	MET
4	2E	12	THR
4	2E	38	THR
4	2E	47	VAL
4	2E	87	GLU
4	2E	116	VAL
4	2E	144	ARG
4	2E	181	LEU
4	2E	184	VAL
5	2F	32	LEU
5	2F	96	ASP
5	2F	107	LYS
5	2F	145	GLU

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Mol	Chain	Res	Type
5	2F	162	LEU
5	2F	165	ARG
5	2F	179	GLU
6	2G	3	LEU
6	2G	4	ASP
6	2G	7	LEU
6	2G	18	GLU
6	2G	28	VAL
6	2G	39	ILE
6	2G	43	LEU
6	2G	51	ARG
6	2G	53	LEU
6	2G	60	LEU
6	2G	91	ARG
6	2G	111	LEU
6	2G	123	ASN
6	2G	140	ILE
6	2G	148	MET
6	2G	152	LEU
6	2G	155	MET
6	2G	168	GLU
6	2G	170	ARG
6	2G	175	LEU
7	2H	23	ARG
7	2H	49	VAL
7	2H	50	VAL
7	2H	70	THR
7	2H	71	LEU
7	2H	81	GLU
7	2H	85	LYS
7	2H	103	LEU
7	2H	122	THR
7	2H	125	VAL
7	2H	129	THR
7	2H	134	SER
7	2H	136	ILE
7	2H	152	ARG
8	2I	14	ASP
8	2I	38	LEU
8	2I	50	ARG
8	2I	58	LEU
8	2I	61	ARG

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Mol	Chain	Res	Type
8	2I	77	LEU
8	2I	82	ARG
8	2I	85	GLU
8	2I	117	GLU
8	2I	125	GLU
8	2I	127	VAL
9	2N	1	MET
9	2N	14	VAL
9	2N	22	THR
9	2N	28	THR
9	2N	48	MET
9	2N	62	VAL
9	2N	63	THR
9	2N	67	LEU
10	2O	21	CYS
10	2O	28	SER
10	2O	52	VAL
10	2O	96	THR
11	2P	7	ARG
11	2P	65	ARG
11	2P	70	GLN
11	2P	96	THR
11	2P	98	GLU
11	2P	117	GLU
11	2P	135	LEU
12	2Q	6	ARG
12	2Q	31	ASP
12	2Q	56	ARG
12	2Q	68	ILE
12	2Q	85	LYS
12	2Q	109	VAL
12	2Q	110	THR
13	2R	6	SER
13	2R	24	GLN
13	2R	67	LEU
13	2R	114	VAL
14	2S	5	THR
14	2S	15	ARG
14	2S	27	SER
14	2S	43	GLU
14	2S	44	LYS
14	2S	53	SER

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Mol	Chain	Res	Type
14	2S	58	LEU
14	2S	63	THR
14	2S	64	GLU
14	2S	78	LEU
14	2S	83	LYS
14	2S	95	HIS
14	2S	98	VAL
15	2T	9	LEU
15	2T	15	VAL
15	2T	50	ILE
15	2T	96	ARG
15	2T	104	ASN
15	2T	107	ASP
15	2T	129	ARG
16	2U	5	LYS
16	2U	31	SER
16	2U	74	LEU
16	2U	85	LYS
16	2U	95	LEU
16	2U	111	GLU
17	2V	1	MET
17	2V	7	THR
17	2V	14	VAL
17	2V	28	GLU
17	2V	56	SER
17	2V	61	VAL
17	2V	79	VAL
17	2V	95	LEU
17	2V	98	GLU
17	2V	100	ARG
18	2W	11	ARG
18	2W	15	ARG
18	2W	67	ASP
19	2X	35	THR
19	2X	48	LYS
19	2X	57	LEU
19	2X	81	VAL
20	2Y	7	VAL
20	2Y	11	ASP
20	2Y	49	VAL
20	2Y	85	VAL
20	2Y	91	GLU

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Mol	Chain	Res	Type
20	2Y	97	ARG
20	2Y	98	VAL
20	2Y	106	LEU
20	2Y	107	ASP
21	2Z	5	LEU
21	2Z	18	LEU
21	2Z	70	LEU
21	2Z	71	VAL
21	2Z	96	VAL
21	2Z	98	MET
21	2Z	121	HIS
21	2Z	122	ARG
21	2Z	123	ASP
21	2Z	145	GLU
21	2Z	154	ASP
21	2Z	155	LEU
21	2Z	161	VAL
21	2Z	170	THR
21	2Z	171	ILE
22	20	7	LEU
22	20	11	ARG
22	20	68	GLU
23	21	46	LEU
23	21	65	SER
23	21	98	LEU
24	22	3	LEU
24	22	11	GLU
24	22	12	GLU
24	22	21	LEU
24	22	66	GLU
24	22	70	GLN
25	23	31	LEU
25	23	56	VAL
26	24	8	LYS
26	24	23	GLU
26	24	24	THR
26	24	34	GLU
26	24	48	ARG
26	24	49	PHE
26	24	56	VAL
26	24	59	PHE
26	24	63	TYR

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Mol	Chain	Res	Type
26	24	67	TYR
26	24	68	ARG
27	25	6	VAL
27	25	55	ARG
27	25	58	LEU
28	26	6	ARG
28	26	23	THR
28	26	32	ASN
29	27	1	MET
29	27	24	THR
29	27	41	ARG
29	27	43	THR
30	28	4	MET
30	28	29	LYS
30	28	31	HIS
30	28	34	TRP
30	28	37	SER
31	29	18	ARG
33	2b	8	LYS
33	2b	10	LEU
33	2b	16	HIS
33	2b	24	TRP
33	2b	47	THR
33	2b	55	PHE
33	2b	60	ASP
33	2b	67	THR
33	2b	68	ILE
33	2b	71	VAL
33	2b	76	GLN
33	2b	94	ASN
33	2b	98	LEU
33	2b	105	PHE
33	2b	112	VAL
33	2b	115	LEU
33	2b	127	ILE
33	2b	164	VAL
33	2b	184	VAL
33	2b	185	ILE
33	2b	189	ASP
33	2b	214	ILE
33	2b	223	ILE
33	2b	229	VAL

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Mol	Chain	Res	Type
33	2b	236	TYR
34	2c	4	LYS
34	2c	18	TRP
34	2c	28	GLN
34	2c	46	GLU
34	2c	47	LEU
34	2c	49	SER
34	2c	52	LEU
34	2c	56	ASP
34	2c	111	LEU
34	2c	115	LEU
34	2c	128	PHE
34	2c	132	ARG
34	2c	140	ARG
34	2c	150	LYS
34	2c	172	ARG
34	2c	190	ARG
35	2d	5	ILE
35	2d	8	VAL
35	2d	31	CYS
35	2d	53	ASP
35	2d	58	LEU
35	2d	76	ARG
35	2d	78	LEU
35	2d	83	SER
35	2d	127	THR
35	2d	135	LEU
35	2d	155	LEU
35	2d	158	ILE
35	2d	170	VAL
35	2d	190	ASP
36	2e	5	ASP
36	2e	10	MET
36	2e	13	ILE
36	2e	31	LEU
36	2e	43	LEU
36	2e	55	VAL
36	2e	66	MET
36	2e	78	HIS
36	2e	115	VAL
36	2e	120	THR
36	2e	125	SER

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Mol	Chain	Res	Type
36	2e	151	LEU
37	2f	19	LEU
37	2f	31	GLU
37	2f	45	LEU
37	2f	63	TYR
37	2f	64	GLN
37	2f	69	GLU
38	2g	13	GLN
38	2g	15	ASP
38	2g	23	VAL
38	2g	38	LEU
38	2g	52	GLU
38	2g	72	ARG
38	2g	78	ARG
38	2g	79	ARG
38	2g	90	GLU
38	2g	106	GLN
38	2g	115	ARG
38	2g	129	GLU
38	2g	142	GLU
38	2g	144	MET
38	2g	146	GLU
38	2g	155	ARG
39	2h	11	THR
39	2h	37	ARG
39	2h	51	VAL
39	2h	52	ASP
39	2h	60	ARG
39	2h	85	ARG
39	2h	86	ILE
39	2h	99	GLU
39	2h	109	ILE
39	2h	112	LEU
39	2h	125	ARG
39	2h	137	VAL
40	2i	14	VAL
40	2i	27	THR
40	2i	50	LEU
40	2i	51	ARG
40	2i	54	ASP
40	2i	65	VAL
40	2i	89	ASN

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Mol	Chain	Res	Type
40	2i	102	LEU
40	2i	103	THR
40	2i	108	VAL
40	2i	113	LYS
41	2j	8	LEU
41	2j	21	GLN
41	2j	65	LEU
41	2j	67	THR
41	2j	89	ASP
41	2j	95	GLU
41	2j	97	GLU
41	2j	100	THR
42	2k	14	VAL
42	2k	24	SER
42	2k	48	ILE
42	2k	87	THR
42	2k	96	ARG
42	2k	105	VAL
42	2k	112	THR
42	2k	114	VAL
42	2k	117	ASN
43	2l	18	VAL
43	2l	33	ARG
43	2l	36	VAL
43	2l	40	VAL
43	2l	83	VAL
43	2l	86	ARG
43	2l	89	ARG
43	2l	117	ARG
44	2m	4	ILE
44	2m	15	VAL
44	2m	32	GLU
44	2m	62	ASN
44	2m	65	LYS
44	2m	67	GLU
44	2m	86	CYS
44	2m	103	THR
44	2m	106	ASN
44	2m	110	ARG
45	2n	18	VAL
45	2n	32	SER
45	2n	33	VAL

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Mol	Chain	Res	Type
45	2n	56	VAL
45	2n	57	ARG
46	2o	5	LYS
46	2o	21	ASP
46	2o	25	THR
46	2o	38	ARG
46	2o	39	LEU
46	2o	76	GLU
46	2o	88	ARG
47	2p	1	MET
47	2p	21	VAL
47	2p	45	THR
47	2p	67	THR
47	2p	74	LEU
48	2q	39	SER
48	2q	41	LYS
48	2q	55	ASP
48	2q	60	ILE
48	2q	63	ARG
48	2q	68	ARG
48	2q	97	SER
49	2r	21	LYS
49	2r	31	LEU
49	2r	54	ARG
49	2r	82	THR
50	2s	5	LEU
50	2s	16	LEU
50	2s	23	ASN
50	2s	33	THR
50	2s	47	HIS
50	2s	48	THR
50	2s	49	ILE
50	2s	81	ARG
50	2s	83	HIS
51	2t	15	ARG
51	2t	46	GLU
51	2t	75	ASN
51	2t	99	LEU
52	2u	7	ARG
52	2u	9	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (115) such sidechains are listed below:

Mol	Chain	Res	Type
4	1E	48	GLN
5	1F	69	HIS
6	1G	26	GLN
6	1G	108	ASN
9	1N	131	GLN
10	1O	3	GLN
10	1O	89	ASN
12	1Q	12	GLN
12	1Q	113	GLN
12	1Q	123	HIS
15	1T	58	ASN
16	1U	81	HIS
19	1X	31	HIS
19	1X	82	GLN
20	1Y	6	HIS
21	1Z	34	ASN
21	1Z	73	GLN
21	1Z	151	HIS
22	10	70	GLN
23	11	56	GLN
25	13	32	GLN
26	14	40	HIS
33	1b	40	HIS
33	1b	78	GLN
33	1b	224	GLN
34	1c	6	HIS
34	1c	37	GLN
34	1c	123	GLN
34	1c	162	GLN
34	1c	181	ASN
35	1d	42	GLN
35	1d	116	GLN
35	1d	123	HIS
35	1d	125	HIS
36	1e	20	GLN
36	1e	78	HIS
36	1e	141	GLN
37	1f	13	ASN
37	1f	57	GLN
37	1f	73	ASN
38	1g	28	ASN
40	1i	31	GLN
40	1i	34	ASN

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Mol	Chain	Res	Type
40	1i	58	HIS
40	1i	89	ASN
40	1i	124	GLN
41	1j	56	HIS
43	1l	99	HIS
44	1m	77	ASN
44	1m	92	HIS
46	1o	46	HIS
48	1q	26	GLN
49	1r	63	GLN
50	1s	57	HIS
50	1s	83	HIS
51	1t	9	ASN
4	2E	48	GLN
5	2F	69	HIS
8	2I	133	HIS
10	2O	5	GLN
11	2P	70	GLN
12	2Q	12	GLN
14	2S	38	GLN
15	2T	58	ASN
16	2U	94	ASN
19	2X	31	HIS
19	2X	82	GLN
21	2Z	34	ASN
21	2Z	55	HIS
21	2Z	73	GLN
21	2Z	151	HIS
22	20	70	GLN
23	21	56	GLN
25	23	32	GLN
33	2b	76	GLN
33	2b	94	ASN
33	2b	135	GLN
34	2c	98	ASN
34	2c	102	ASN
34	2c	136	GLN
35	2d	77	ASN
35	2d	116	GLN
35	2d	119	GLN
35	2d	123	HIS
35	2d	125	HIS

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Mol	Chain	Res	Type
35	2d	160	GLN
36	2e	38	GLN
36	2e	73	ASN
36	2e	78	HIS
36	2e	130	ASN
37	2f	73	ASN
37	2f	100	ASN
38	2g	28	ASN
38	2g	86	GLN
38	2g	106	GLN
40	2i	3	GLN
40	2i	31	GLN
40	2i	58	HIS
41	2j	21	GLN
41	2j	33	GLN
41	2j	69	ASN
42	2k	78	GLN
42	2k	104	GLN
42	2k	117	ASN
43	2l	99	HIS
44	2m	62	ASN
44	2m	77	ASN
48	2q	93	GLN
49	2r	63	GLN
50	2s	23	ASN
50	2s	47	HIS
50	2s	69	HIS
50	2s	83	HIS
51	2t	75	ASN
51	2t	90	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2863/2915 (98%)	432 (15%)	25 (0%)
1	2A	2790/2915 (95%)	463 (16%)	25 (0%)
2	1B	119/121 (98%)	8 (6%)	0
2	2B	118/121 (97%)	27 (22%)	0
32	1a	1494/1521 (98%)	233 (15%)	0
32	2a	1498/1521 (98%)	299 (19%)	0
53	1v	12/24 (50%)	1 (8%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
53	2v	12/24 (50%)	1 (8%)	0
54	1w	68/76 (89%)	20 (29%)	0
54	2w	65/76 (85%)	16 (24%)	0
55	1x	74/77 (96%)	8 (10%)	0
55	2x	74/77 (96%)	9 (12%)	0
56	1y	71/76 (93%)	24 (33%)	0
56	2y	69/76 (90%)	17 (24%)	0
All	All	9327/9620 (96%)	1558 (16%)	50 (0%)

All (1558) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	10	G
1	1A	12	U
1	1A	34	C
1	1A	36	G
1	1A	45	C
1	1A	71	A
1	1A	74	A
1	1A	75	G
1	1A	84	A
1	1A	118	A
1	1A	119	A
1	1A	120	U
1	1A	154(A)	C
1	1A	196	A
1	1A	199	A
1	1A	205	G
1	1A	214	G
1	1A	215	G
1	1A	216	A
1	1A	222	A
1	1A	228	A
1	1A	229	A
1	1A	233	A
1	1A	248	G
1	1A	269	U
1	1A	271(K)	U
1	1A	271(L)	U
1	1A	271(M)	G
1	1A	271(O)	C
1	1A	271(S)	G

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Mol	Chain	Res	Type
1	1A	272(A)	U
1	1A	272(B)	G
1	1A	272(H)	C
1	1A	274	G
1	1A	275	G
1	1A	279	C
1	1A	311	A
1	1A	329	G
1	1A	330	A
1	1A	352	G
1	1A	363	G
1	1A	363(A)	A
1	1A	363(B)	G
1	1A	380	U
1	1A	386	G
1	1A	396	G
1	1A	405	U
1	1A	411	G
1	1A	428	A
1	1A	444	C
1	1A	448	U
1	1A	451	C
1	1A	454	A
1	1A	455	C
1	1A	456	C
1	1A	457	A
1	1A	479	A
1	1A	481	G
1	1A	494	G
1	1A	504	U
1	1A	505	A
1	1A	509	C
1	1A	530	G
1	1A	531	C
1	1A	532	A
1	1A	533	G
1	1A	545	G
1	1A	549	G
1	1A	563	G
1	1A	573	G
1	1A	575	A
1	1A	586	A

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Mol	Chain	Res	Type
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	616	G
1	1A	627	A
1	1A	637	A
1	1A	645	C
1	1A	646	A
1	1A	652(A)	A
1	1A	652(D)	C
1	1A	652(E)	G
1	1A	652(F)	G
1	1A	652(T)	C
1	1A	669	G
1	1A	686	G
1	1A	730	C
1	1A	740	U
1	1A	764	A
1	1A	775	G
1	1A	776	G
1	1A	782	A
1	1A	783	A
1	1A	784	A
1	1A	785	G
1	1A	789	A
1	1A	790	C
1	1A	792	G
1	1A	805	G
1	1A	812	C
1	1A	819	A
1	1A	824	A
1	1A	827	U
1	1A	828	U
1	1A	855	G
1	1A	859	G
1	1A	866	A
1	1A	879	G
1	1A	880	G

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Mol	Chain	Res	Type
1	1A	882	G
1	1A	883	G
1	1A	884	C
1	1A	885	C
1	1A	886	C
1	1A	887	A
1	1A	888	C
1	1A	889	C
1	1A	890	A
1	1A	894	C
1	1A	895	U
1	1A	896	A
1	1A	897	C
1	1A	898	C
1	1A	907	U
1	1A	910	A
1	1A	915	C
1	1A	932	G
1	1A	945	A
1	1A	946	G
1	1A	953	A
1	1A	959	A
1	1A	961	C
1	1A	974	G
1	1A	975	C
1	1A	983	A
1	1A	996	A
1	1A	1005	C
1	1A	1012	U
1	1A	1013	C
1	1A	1025	G
1	1A	1026	U
1	1A	1033	U
1	1A	1038	C
1	1A	1041	C
1	1A	1043	C
1	1A	1045	A
1	1A	1046	A
1	1A	1047	G
1	1A	1054	A
1	1A	1055	G
1	1A	1057	A

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Mol	Chain	Res	Type
1	1A	1058	G
1	1A	1059	G
1	1A	1063	G
1	1A	1066	U
1	1A	1069	A
1	1A	1070	A
1	1A	1071	G
1	1A	1073	A
1	1A	1075	C
1	1A	1076	C
1	1A	1078	U
1	1A	1079	C
1	1A	1081	U
1	1A	1083	U
1	1A	1087	G
1	1A	1088	A
1	1A	1089	G
1	1A	1090	U
1	1A	1091	G
1	1A	1093	G
1	1A	1094	U
1	1A	1099	G
1	1A	1100	C
1	1A	1101	U
1	1A	1110	G
1	1A	1111	A
1	1A	1112	G
1	1A	1115	G
1	1A	1116	C
1	1A	1117	G
1	1A	1128	A
1	1A	1130	U
1	1A	1135	C
1	1A	1136	G
1	1A	1171	G
1	1A	1173	G
1	1A	1174	A
1	1A	1175	U
1	1A	1176	G
1	1A	1177	A
1	1A	1178	C
1	1A	1220	A

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Mol	Chain	Res	Type
1	1A	1253	A
1	1A	1256	G
1	1A	1271	G
1	1A	1272	A
1	1A	1273	U
1	1A	1300	U
1	1A	1301	A
1	1A	1303	G
1	1A	1345	C
1	1A	1352	U
1	1A	1359	A
1	1A	1360	A
1	1A	1365	A
1	1A	1380	G
1	1A	1384	A
1	1A	1385	G
1	1A	1386	C
1	1A	1416	G
1	1A	1417	C
1	1A	1420	U
1	1A	1421	G
1	1A	1428	C
1	1A	1445	A
1	1A	1450	G
1	1A	1455	G
1	1A	1461	G
1	1A	1467	C
1	1A	1473	G
1	1A	1482	G
1	1A	1493	C
1	1A	1494	A
1	1A	1508	A
1	1A	1509	C
1	1A	1509(A)	A
1	1A	1532	C
1	1A	1540	U
1	1A	1541	G
1	1A	1543	C
1	1A	1554	A
1	1A	1558	A
1	1A	1566	A
1	1A	1569	A

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Mol	Chain	Res	Type
1	1A	1578	U
1	1A	1581	G
1	1A	1584	C
1	1A	1586	A
1	1A	1608	A
1	1A	1609	A
1	1A	1610	A
1	1A	1647	G
1	1A	1648	C
1	1A	1674	G
1	1A	1700	A
1	1A	1701	A
1	1A	1703	G
1	1A	1722	A
1	1A	1739	U
1	1A	1746	G
1	1A	1756	G
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	1816	G
1	1A	1828	G
1	1A	1847	A
1	1A	1861	G
1	1A	1877	A
1	1A	1878	G
1	1A	1889	A
1	1A	1900	A
1	1A	1906	G
1	1A	1929	G
1	1A	1930	G
1	1A	1938	A
1	1A	1955	U
1	1A	1963	U
1	1A	1967	C
1	1A	1970	A
1	1A	1971	A

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Mol	Chain	Res	Type
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	2062	A
1	1A	2069	G
1	1A	2098	U
1	1A	2101	G
1	1A	2108	C
1	1A	2110	G
1	1A	2112	G
1	1A	2113	U
1	1A	2116	G
1	1A	2119	A
1	1A	2121	G
1	1A	2122	U
1	1A	2126	A
1	1A	2127	G
1	1A	2129	C
1	1A	2130	U
1	1A	2131	G
1	1A	2132	U
1	1A	2133	G
1	1A	2134	A
1	1A	2135	A
1	1A	2136	C
1	1A	2140	C
1	1A	2142	C
1	1A	2143	C
1	1A	2144	U
1	1A	2146	C
1	1A	2147	G
1	1A	2150	U

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Mol	Chain	Res	Type
1	1A	2151	G
1	1A	2156	G
1	1A	2157	G
1	1A	2158	A
1	1A	2159	G
1	1A	2165	G
1	1A	2166	G
1	1A	2168	G
1	1A	2171	A
1	1A	2172	U
1	1A	2173	A
1	1A	2174	C
1	1A	2182	G
1	1A	2184	G
1	1A	2189	U
1	1A	2192	G
1	1A	2198	A
1	1A	2206	G
1	1A	2207	G
1	1A	2208	A
1	1A	2218	U
1	1A	2219	G
1	1A	2225	A
1	1A	2235	G
1	1A	2238	G
1	1A	2239	G
1	1A	2268	A
1	1A	2269	A
1	1A	2273	A
1	1A	2283	C
1	1A	2287	A
1	1A	2305	A
1	1A	2307	G
1	1A	2308	G
1	1A	2312	U
1	1A	2313	C
1	1A	2320	A
1	1A	2325	G
1	1A	2334	G
1	1A	2336	A
1	1A	2347	C
1	1A	2354	G

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Mol	Chain	Res	Type
1	1A	2361	A
1	1A	2379	G
1	1A	2383	G
1	1A	2385	C
1	1A	2405	G
1	1A	2406	U
1	1A	2422	A
1	1A	2423	U
1	1A	2425	A
1	1A	2429	G
1	1A	2430	A
1	1A	2431	U
1	1A	2435	A
1	1A	2439	A
1	1A	2441	C
1	1A	2448	A
1	1A	2474	C
1	1A	2476	A
1	1A	2478	A
1	1A	2502	G
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	2573	C
1	1A	2578	G
1	1A	2602	A
1	1A	2609	U
1	1A	2611	U
1	1A	2612	C
1	1A	2629	A
1	1A	2630	G
1	1A	2654	A
1	1A	2689	U
1	1A	2690	C
1	1A	2691	C
1	1A	2702	U
1	1A	2703	C
1	1A	2712(A)	A

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Mol	Chain	Res	Type
1	1A	2713	A
1	1A	2714	G
1	1A	2726	U
1	1A	2733	A
1	1A	2758	A
1	1A	2764	A
1	1A	2765	A
1	1A	2778	A
1	1A	2790	A
1	1A	2791	C
1	1A	2792	G
1	1A	2793	G
1	1A	2794	C
1	1A	2802	G
1	1A	2804	C
1	1A	2810	A
1	1A	2820	A
1	1A	2821	A
1	1A	2835	A
1	1A	2872	G
1	1A	2880	C
1	1A	2892	A
1	1A	2894	G
1	1A	2895	U
2	1B	12	C
2	1B	32	C
2	1B	35	U
2	1B	56	G
2	1B	57	A
2	1B	73	A
2	1B	85	G
2	1B	110	G
32	1a	7	G
32	1a	9	G
32	1a	32	A
32	1a	39	G
32	1a	47	C
32	1a	48	C
32	1a	51	A
32	1a	52	G
32	1a	61	G
32	1a	70	G

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Mol	Chain	Res	Type
32	1a	79	G
32	1a	91	C
32	1a	98	G
32	1a	101	A
32	1a	105	G
32	1a	116	A
32	1a	120	A
32	1a	121	C
32	1a	131	C
32	1a	145	G
32	1a	147	G
32	1a	162	A
32	1a	163	C
32	1a	174	C
32	1a	182	U
32	1a	189(J)	G
32	1a	195	A
32	1a	197	A
32	1a	199	G
32	1a	201	C
32	1a	202	U
32	1a	203	U
32	1a	204	U
32	1a	222	U
32	1a	247	G
32	1a	251	G
32	1a	266	G
32	1a	267	C
32	1a	289	G
32	1a	318	G
32	1a	328	C
32	1a	329	A
32	1a	332	G
32	1a	342	C
32	1a	348	G
32	1a	351	G
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	367	U
32	1a	372	C
32	1a	373	A

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Mol	Chain	Res	Type
32	1a	384	G
32	1a	397	A
32	1a	398	C
32	1a	406	G
32	1a	412	A
32	1a	413	G
32	1a	414	A
32	1a	422	C
32	1a	423	G
32	1a	424	G
32	1a	429	U
32	1a	439	A
32	1a	442	C
32	1a	452	A
32	1a	461	A
32	1a	470	C
32	1a	471	G
32	1a	474	G
32	1a	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	527	7MG
32	1a	531	U
32	1a	532	A
32	1a	547	A
32	1a	559	A
32	1a	561	U
32	1a	568	G
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	577	G
32	1a	596	C
32	1a	628	G
32	1a	630	G
32	1a	653	A

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Mol	Chain	Res	Type
32	1a	665	A
32	1a	687	A
32	1a	688	G
32	1a	695	A
32	1a	723	U
32	1a	724	G
32	1a	731	G
32	1a	749	C
32	1a	752	G
32	1a	753	A
32	1a	755	G
32	1a	766	A
32	1a	777	A
32	1a	792	A
32	1a	793	U
32	1a	794	A
32	1a	815	A
32	1a	817	C
32	1a	821	G
32	1a	827	U
32	1a	828	A
32	1a	840	C
32	1a	841	U
32	1a	851	G
32	1a	870	U
32	1a	874	G
32	1a	876	G
32	1a	877	C
32	1a	914	A
32	1a	916	G
32	1a	926	G
32	1a	927	G
32	1a	934	C
32	1a	942	G
32	1a	958	A
32	1a	960	U
32	1a	961	U
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	972	C
32	1a	974	A

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Mol	Chain	Res	Type
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	983	A
32	1a	992	U
32	1a	993	G
32	1a	997	U
32	1a	1000	U
32	1a	1003	G
32	1a	1005	A
32	1a	1006	C
32	1a	1020	U
32	1a	1022	G
32	1a	1023	G
32	1a	1025	U
32	1a	1026	G
32	1a	1027	C
32	1a	1028	C
32	1a	1029	C
32	1a	1030	C
32	1a	1030(A)	G
32	1a	1030(C)	G
32	1a	1031	G
32	1a	1039	C
32	1a	1044	A
32	1a	1045	C
32	1a	1053	G
32	1a	1068	G
32	1a	1081	G
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1121	U
32	1a	1123	A
32	1a	1125	U
32	1a	1134	G
32	1a	1137	C
32	1a	1138	G
32	1a	1139	G
32	1a	1146	A
32	1a	1152	A
32	1a	1159	U

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Mol	Chain	Res	Type
32	1a	1183	A
32	1a	1184	G
32	1a	1196	U
32	1a	1197	G
32	1a	1202	G
32	1a	1214	C
32	1a	1227	A
32	1a	1236	A
32	1a	1238	A
32	1a	1250	A
32	1a	1256	A
32	1a	1257	U
32	1a	1260	C
32	1a	1270	C
32	1a	1275	A
32	1a	1276	G
32	1a	1278	U
32	1a	1279	A
32	1a	1280	A
32	1a	1286	A
32	1a	1287	A
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1305	G
32	1a	1312	G
32	1a	1320	C
32	1a	1322	C
32	1a	1338	G
32	1a	1340	A
32	1a	1346	A
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1370	G
32	1a	1378	C
32	1a	1381	U
32	1a	1397	C
32	1a	1419	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1446	U

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Mol	Chain	Res	Type
32	1a	1447	A
32	1a	1456	G
32	1a	1487	G
32	1a	1492	A
32	1a	1494	G
32	1a	1497	G
32	1a	1503	A
32	1a	1504	G
32	1a	1506	U
32	1a	1517	G
32	1a	1529	G
32	1a	1530	G
32	1a	1532	U
53	1v	13	A
54	1w	2	C
54	1w	7	A
54	1w	8	4SU
54	1w	14	A
54	1w	19	G
54	1w	20	U
54	1w	21	A
54	1w	23	A
54	1w	24	G
54	1w	45	U
54	1w	46	7MG
54	1w	47	U
54	1w	48	C
54	1w	50	U
54	1w	62	C
54	1w	63	G
54	1w	64	A
54	1w	68	C
54	1w	70	G
54	1w	73	A
55	1x	9	G
55	1x	14	A
55	1x	18	G
55	1x	19	G
55	1x	21	A
55	1x	38	A
55	1x	47	U
55	1x	61	C

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Mol	Chain	Res	Type
56	1y	6	G
56	1y	8	4SU
56	1y	9	A
56	1y	13	C
56	1y	14	A
56	1y	15	G
56	1y	19	G
56	1y	20	U
56	1y	21	A
56	1y	35	A
56	1y	36	A
56	1y	44	G
56	1y	45	U
56	1y	46	7MG
56	1y	48	C
56	1y	53	G
56	1y	54	5MU
56	1y	56	C
56	1y	57	G
56	1y	59	U
56	1y	64	A
56	1y	65	G
56	1y	69	G
56	1y	70	G
1	2A	8	A
1	2A	15	G
1	2A	16	G
1	2A	34	C
1	2A	35	G
1	2A	45	C
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	79	G
1	2A	84	A
1	2A	90	U
1	2A	94	C
1	2A	95	G
1	2A	100	G
1	2A	102	G
1	2A	118	A
1	2A	119	A

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Mol	Chain	Res	Type
1	2A	120	U
1	2A	125	G
1	2A	154(A)	C
1	2A	157	U
1	2A	173	G
1	2A	181	A
1	2A	196	A
1	2A	199	A
1	2A	205	G
1	2A	214	G
1	2A	215	G
1	2A	216	A
1	2A	221	A
1	2A	222	A
1	2A	225	A
1	2A	228	A
1	2A	229	A
1	2A	230	U
1	2A	232	G
1	2A	233	A
1	2A	248	G
1	2A	250	G
1	2A	264	C
1	2A	271(K)	U
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	272(B)	G
1	2A	277	C
1	2A	278	A
1	2A	304	G
1	2A	311	A
1	2A	317	G
1	2A	324	A
1	2A	327	G
1	2A	329	G
1	2A	330	A
1	2A	333	G
1	2A	352	G
1	2A	354	G
1	2A	363	G
1	2A	363(B)	G

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Mol	Chain	Res	Type
1	2A	363(E)	U
1	2A	372	G
1	2A	380	U
1	2A	386	G
1	2A	399	G
1	2A	403	U
1	2A	411	G
1	2A	421	U
1	2A	422	A
1	2A	444	C
1	2A	454	A
1	2A	455	C
1	2A	457	A
1	2A	481	G
1	2A	503	A
1	2A	504	U
1	2A	505	A
1	2A	509	C
1	2A	529	A
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	533	G
1	2A	545	G
1	2A	562	U
1	2A	563	G
1	2A	568	U
1	2A	573	G
1	2A	575	A
1	2A	588	U
1	2A	599	G
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	614(B)	G
1	2A	615	G
1	2A	616	G
1	2A	626	U
1	2A	627	A
1	2A	634	C
1	2A	637	A
1	2A	645	C

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Mol	Chain	Res	Type
1	2A	652(B)	A
1	2A	652(C)	G
1	2A	669	G
1	2A	686	G
1	2A	715	G
1	2A	717	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	790	C
1	2A	792	G
1	2A	805	G
1	2A	812	C
1	2A	819	A
1	2A	827	U
1	2A	828	U
1	2A	832	G
1	2A	857	C
1	2A	859	G
1	2A	874	G
1	2A	877	U
1	2A	878	A
1	2A	879	G
1	2A	880	G
1	2A	884	C
1	2A	886	C
1	2A	887	A
1	2A	888	C
1	2A	889	C
1	2A	893	C
1	2A	894	C
1	2A	896	A
1	2A	900	A
1	2A	901	A
1	2A	910	A

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Mol	Chain	Res	Type
1	2A	914	C
1	2A	917	A
1	2A	919	G
1	2A	932	G
1	2A	941	A
1	2A	945	A
1	2A	946	G
1	2A	953	A
1	2A	959	A
1	2A	961	C
1	2A	974	G
1	2A	975	C
1	2A	983	A
1	2A	996	A
1	2A	997	G
1	2A	999	U
1	2A	1012	U
1	2A	1013	C
1	2A	1017	G
1	2A	1021	A
1	2A	1022	G
1	2A	1023	U
1	2A	1025	G
1	2A	1026	U
1	2A	1027	A
1	2A	1033	U
1	2A	1038	C
1	2A	1039	G
1	2A	1041	C
1	2A	1043	C
1	2A	1114	G
1	2A	1116	C
1	2A	1126	A
1	2A	1130	U
1	2A	1133	U
1	2A	1135	C
1	2A	1136	G
1	2A	1139	G
1	2A	1142(A)	A
1	2A	1169	G
1	2A	1171	G
1	2A	1210	A

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Mol	Chain	Res	Type
1	2A	1211	U
1	2A	1212	G
1	2A	1220	A
1	2A	1221	C
1	2A	1229	G
1	2A	1241	A
1	2A	1242	A
1	2A	1244	G
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	1303	G
1	2A	1314	C
1	2A	1352	U
1	2A	1359	A
1	2A	1360	A
1	2A	1365	A
1	2A	1368	G
1	2A	1370	C
1	2A	1373	A
1	2A	1379	A
1	2A	1380	G
1	2A	1384	A
1	2A	1385	G
1	2A	1386	C
1	2A	1416	G
1	2A	1417	C
1	2A	1421	G
1	2A	1427	A
1	2A	1428	C
1	2A	1437	C
1	2A	1445	A
1	2A	1449	A
1	2A	1450	G
1	2A	1460	A
1	2A	1466	G
1	2A	1467	C

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Mol	Chain	Res	Type
1	2A	1471	A
1	2A	1482	G
1	2A	1490	A
1	2A	1493	C
1	2A	1496	A
1	2A	1497	U
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1531	C
1	2A	1532	C
1	2A	1533	G
1	2A	1547	C
1	2A	1558	A
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1583	A
1	2A	1584	C
1	2A	1586	A
1	2A	1608	A
1	2A	1609	A
1	2A	1610	A
1	2A	1616	A
1	2A	1647	G
1	2A	1648	C
1	2A	1654	A
1	2A	1664	A
1	2A	1674	G
1	2A	1696	G
1	2A	1700	A
1	2A	1701	A
1	2A	1703	G
1	2A	1721	G
1	2A	1722	A
1	2A	1740	G
1	2A	1746	G
1	2A	1756	G
1	2A	1762	A
1	2A	1763	G
1	2A	1764	G
1	2A	1773	A

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Mol	Chain	Res	Type
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	1829	A
1	2A	1835	G
1	2A	1847	A
1	2A	1848	A
1	2A	1877	A
1	2A	1878	G
1	2A	1889	A
1	2A	1900	A
1	2A	1906	G
1	2A	1914	C
1	2A	1929	G
1	2A	1930	G
1	2A	1936	A
1	2A	1938	A
1	2A	1955	U
1	2A	1963	U
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	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	2106	G

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Mol	Chain	Res	Type
1	2A	2110	G
1	2A	2111	C
1	2A	2113	U
1	2A	2116	G
1	2A	2117	A
1	2A	2120	G
1	2A	2122	U
1	2A	2124	G
1	2A	2125	G
1	2A	2126	A
1	2A	2127	G
1	2A	2128	C
1	2A	2131	G
1	2A	2132	U
1	2A	2133	G
1	2A	2134	A
1	2A	2135	A
1	2A	2137	C
1	2A	2138	C
1	2A	2139	C
1	2A	2140	C
1	2A	2141	G
1	2A	2142	C
1	2A	2146	C
1	2A	2150	U
1	2A	2156	G
1	2A	2157	G
1	2A	2158	A
1	2A	2159	G
1	2A	2161	C
1	2A	2165	G
1	2A	2166	G
1	2A	2167	U
1	2A	2168	G
1	2A	2170	A
1	2A	2172	U
1	2A	2174	C
1	2A	2176	A
1	2A	2178	C
1	2A	2182	G
1	2A	2185	C
1	2A	2189	U

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Mol	Chain	Res	Type
1	2A	2192	G
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2218	U
1	2A	2225	A
1	2A	2239	G
1	2A	2269	A
1	2A	2275	C
1	2A	2278	A
1	2A	2280	G
1	2A	2283	C
1	2A	2287	A
1	2A	2288	A
1	2A	2298	A
1	2A	2305	A
1	2A	2308	G
1	2A	2312	U
1	2A	2315	G
1	2A	2319	G
1	2A	2320	A
1	2A	2325	G
1	2A	2327	A
1	2A	2334	G
1	2A	2336	A
1	2A	2341	G
1	2A	2346	A
1	2A	2347	C
1	2A	2350	C
1	2A	2354	G
1	2A	2376	A
1	2A	2379	G
1	2A	2383	G
1	2A	2385	C
1	2A	2388	A
1	2A	2403	C
1	2A	2406	U
1	2A	2425	A
1	2A	2429	G
1	2A	2430	A
1	2A	2434	A

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Mol	Chain	Res	Type
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2445	G
1	2A	2448	A
1	2A	2460	U
1	2A	2465	C
1	2A	2469	A
1	2A	2476	A
1	2A	2490	G
1	2A	2491	U
1	2A	2494	G
1	2A	2502	G
1	2A	2505	G
1	2A	2506	U
1	2A	2507	C
1	2A	2518	A
1	2A	2520	C
1	2A	2525	G
1	2A	2529	G
1	2A	2534	A
1	2A	2554	U
1	2A	2555	U
1	2A	2566	A
1	2A	2567	G
1	2A	2573	C
1	2A	2577	A
1	2A	2578	G
1	2A	2602	A
1	2A	2609	U
1	2A	2611	U
1	2A	2612	C
1	2A	2630	G
1	2A	2634	G
1	2A	2652	C
1	2A	2654	A
1	2A	2673	G
1	2A	2689	U
1	2A	2690	C
1	2A	2702	U
1	2A	2703	C
1	2A	2712(A)	A

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Mol	Chain	Res	Type
1	2A	2713	A
1	2A	2714	G
1	2A	2718	G
1	2A	2726	U
1	2A	2733	A
1	2A	2751	G
1	2A	2757	A
1	2A	2758	A
1	2A	2761	G
1	2A	2764	A
1	2A	2765	A
1	2A	2766	G
1	2A	2778	A
1	2A	2789	C
1	2A	2793	G
1	2A	2803	C
1	2A	2820	A
1	2A	2821	A
1	2A	2835	A
1	2A	2850	A
1	2A	2872	G
1	2A	2880	C
1	2A	2892	A
1	2A	2894	G
1	2A	2897	U
2	2B	2	C
2	2B	8	U
2	2B	12	C
2	2B	17	C
2	2B	19	G
2	2B	33	G
2	2B	34	U
2	2B	35	U
2	2B	38	C
2	2B	41	U
2	2B	42	C
2	2B	56	G
2	2B	58	A
2	2B	67	G
2	2B	69	G
2	2B	73	A
2	2B	74	U

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Mol	Chain	Res	Type
2	2B	75	G
2	2B	84	C
2	2B	85	G
2	2B	89	G
2	2B	106	G
2	2B	108	U
2	2B	110	G
2	2B	111	G
2	2B	116	G
2	2B	120	A
32	2a	9	G
32	2a	16	A
32	2a	22	G
32	2a	26	A
32	2a	32	A
32	2a	39	G
32	2a	47	C
32	2a	48	C
32	2a	50	A
32	2a	51	A
32	2a	54	C
32	2a	65	U
32	2a	66	G
32	2a	73	G
32	2a	88	A
32	2a	89	C
32	2a	101	A
32	2a	116	A
32	2a	121	C
32	2a	131	C
32	2a	142	G
32	2a	143	A
32	2a	159	G
32	2a	163	C
32	2a	182	U
32	2a	189(F)	U
32	2a	195	A
32	2a	197	A
32	2a	202	U
32	2a	203	U
32	2a	204	U
32	2a	216	G

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Mol	Chain	Res	Type
32	2a	217	C
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	289	G
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	349	A
32	2a	351	G
32	2a	352	C
32	2a	353	A
32	2a	354	G
32	2a	367	U
32	2a	372	C
32	2a	373	A
32	2a	384	G
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	412	A
32	2a	413	G
32	2a	414	A
32	2a	421	U
32	2a	423	G
32	2a	424	G
32	2a	429	U
32	2a	430	A
32	2a	441	A
32	2a	442	C
32	2a	452	A
32	2a	461	A
32	2a	470	C
32	2a	471	G
32	2a	484	G
32	2a	485	G
32	2a	496	A
32	2a	498	U
32	2a	499	A

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Mol	Chain	Res	Type
32	2a	505	G
32	2a	509	A
32	2a	510	A
32	2a	511	C
32	2a	517	G
32	2a	518	C
32	2a	521	G
32	2a	527	7MG
32	2a	531	U
32	2a	532	A
32	2a	533	A
32	2a	547	A
32	2a	559	A
32	2a	562	C
32	2a	564	C
32	2a	572	A
32	2a	573	A
32	2a	574	A
32	2a	575	G
32	2a	576	G
32	2a	596	C
32	2a	607	A
32	2a	630	G
32	2a	653	A
32	2a	657	G
32	2a	665	A
32	2a	687	A
32	2a	688	G
32	2a	695	A
32	2a	702	A
32	2a	703	G
32	2a	720	C
32	2a	721	G
32	2a	723	U
32	2a	731	G
32	2a	742	G
32	2a	748	C
32	2a	749	C
32	2a	755	G
32	2a	760	G
32	2a	774	G
32	2a	777	A

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Mol	Chain	Res	Type
32	2a	787	A
32	2a	792	A
32	2a	793	U
32	2a	794	A
32	2a	805	C
32	2a	816	A
32	2a	817	C
32	2a	821	G
32	2a	828	A
32	2a	840	C
32	2a	841	U
32	2a	853	G
32	2a	855	G
32	2a	859	A
32	2a	871	U
32	2a	872	A
32	2a	887	G
32	2a	902	G
32	2a	914	A
32	2a	926	G
32	2a	927	G
32	2a	932	C
32	2a	934	C
32	2a	935	A
32	2a	942	G
32	2a	958	A
32	2a	960	U
32	2a	961	U
32	2a	963	G
32	2a	968	A
32	2a	969	A
32	2a	971	G
32	2a	974	A
32	2a	975	A
32	2a	976	G
32	2a	977	A
32	2a	984	C
32	2a	992	U
32	2a	993	G
32	2a	994	A
32	2a	995	C
32	2a	997	U

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Mol	Chain	Res	Type
32	2a	999	C
32	2a	1001	A
32	2a	1002	G
32	2a	1003	G
32	2a	1004	A
32	2a	1005	A
32	2a	1006	C
32	2a	1009	G
32	2a	1011	G
32	2a	1012	U
32	2a	1016	A
32	2a	1017	G
32	2a	1020	U
32	2a	1021	G
32	2a	1022	G
32	2a	1023	G
32	2a	1025	U
32	2a	1026	G
32	2a	1027	C
32	2a	1028	C
32	2a	1029	C
32	2a	1030	C
32	2a	1030(A)	G
32	2a	1031	G
32	2a	1033	G
32	2a	1035	A
32	2a	1039	C
32	2a	1040	U
32	2a	1046	A
32	2a	1050	G
32	2a	1051	C
32	2a	1052	U
32	2a	1053	G
32	2a	1054	C
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1077	G
32	2a	1078	U
32	2a	1079	G
32	2a	1081	G
32	2a	1086	U

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Mol	Chain	Res	Type
32	2a	1092	A
32	2a	1093	A
32	2a	1094	G
32	2a	1095	U
32	2a	1101	A
32	2a	1105	A
32	2a	1108	G
32	2a	1109	C
32	2a	1113	C
32	2a	1122	U
32	2a	1124	G
32	2a	1125	U
32	2a	1129	C
32	2a	1130	A
32	2a	1132	C
32	2a	1133	G
32	2a	1136	U
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G
32	2a	1146	A
32	2a	1147	C
32	2a	1149	C
32	2a	1152	A
32	2a	1157	A
32	2a	1158	C
32	2a	1159	U
32	2a	1172	C
32	2a	1182	G
32	2a	1184	G
32	2a	1191	A
32	2a	1196	U
32	2a	1197	G
32	2a	1202	G
32	2a	1207	2MG
32	2a	1211	U
32	2a	1212	U
32	2a	1213	A
32	2a	1219	U
32	2a	1227	A
32	2a	1236	A
32	2a	1238	A

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Mol	Chain	Res	Type
32	2a	1240	U
32	2a	1241	G
32	2a	1246	C
32	2a	1256	A
32	2a	1257	U
32	2a	1260	C
32	2a	1261	A
32	2a	1262	C
32	2a	1264	C
32	2a	1270	C
32	2a	1272	G
32	2a	1273	G
32	2a	1277	C
32	2a	1279	A
32	2a	1280	A
32	2a	1283	G
32	2a	1287	A
32	2a	1293	G
32	2a	1294	G
32	2a	1299	A
32	2a	1300	G
32	2a	1302	U
32	2a	1303	C
32	2a	1305	G
32	2a	1306	A
32	2a	1313	U
32	2a	1320	C
32	2a	1323	G
32	2a	1336	C
32	2a	1346	A
32	2a	1347	G
32	2a	1350	A
32	2a	1354	C
32	2a	1363	C
32	2a	1364	U
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

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Mol	Chain	Res	Type
32	2a	1442(B)	A
32	2a	1447	A
32	2a	1452	C
32	2a	1456	G
32	2a	1492	A
32	2a	1494	G
32	2a	1497	G
32	2a	1504	G
32	2a	1506	U
32	2a	1507	A
32	2a	1517	G
32	2a	1529	G
32	2a	1530	G
32	2a	1531	A
32	2a	1532	U
53	2v	13	A
54	2w	3	C
54	2w	4	C
54	2w	11	C
54	2w	13	C
54	2w	14	A
54	2w	19	G
54	2w	22	G
54	2w	46	7MG
54	2w	47	U
54	2w	48	C
54	2w	62	C
54	2w	63	G
54	2w	69	G
54	2w	70	G
54	2w	71	G
54	2w	73	A
55	2x	9	G
55	2x	13	C
55	2x	18	G
55	2x	19	G
55	2x	21	A
55	2x	42	G
55	2x	47	U
55	2x	59	A
55	2x	61	C
56	2y	2	C

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Mol	Chain	Res	Type
56	2y	15	G
56	2y	19	G
56	2y	25	C
56	2y	26	A
56	2y	27	G
56	2y	45	U
56	2y	48	C
56	2y	49	C
56	2y	52	G
56	2y	53	G
56	2y	54	5MU
56	2y	56	C
56	2y	58	A
56	2y	60	U
56	2y	69	G
56	2y	70	G

All (50) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	195	A
1	1A	196	A
1	1A	266	G
1	1A	278	A
1	1A	548	A
1	1A	746	A
1	1A	774	A
1	1A	974	G
1	1A	1067	A
1	1A	1142(A)	A
1	1A	1174	A
1	1A	1176	G
1	1A	1379	A
1	1A	1442	G
1	1A	1508	A
1	1A	1608	A
1	1A	1992	G
1	1A	2134	A
1	1A	2181	G
1	1A	2183	C
1	1A	2406	U
1	1A	2422	A

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Mol	Chain	Res	Type
1	1A	2430	A
1	1A	2629	A
1	1A	2689	U
1	2A	196	A
1	2A	228	A
1	2A	266	G
1	2A	271(M)	G
1	2A	277	C
1	2A	528	A
1	2A	752	A
1	2A	774	A
1	2A	827	U
1	2A	856	C
1	2A	900	A
1	2A	1026	U
1	2A	1210	A
1	2A	1240	U
1	2A	1379	A
1	2A	1420	U
1	2A	1442	G
1	2A	1530	C
1	2A	1653	G
1	2A	1913	A
1	2A	1992	G
1	2A	2119	A
1	2A	2126	A
1	2A	2689	U
1	2A	2756	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	5MC	2a	1407	32	15,22,23	1.36	1 (6%)	19,32,35	1.38	3 (15%)
32	5MC	1a	967	32	15,22,23	1.29	1 (6%)	19,32,35	1.33	2 (10%)
56	PSU	2y	39	56	17,21,22	1.53	2 (11%)	20,30,33	3.36	6 (30%)
54	4SU	1w	8	54	14,21,22	1.32	1 (7%)	15,30,33	1.49	2 (13%)
32	4OC	1a	1402	32	16,23,24	0.63	0	17,32,35	0.95	0
1	OMU	1A	2552	57,1	14,22,23	0.87	0	14,31,34	0.74	1 (7%)
56	4SU	1y	8	56	14,21,22	1.36	2 (14%)	15,30,33	1.43	2 (13%)
32	PSU	2a	516	32	17,21,22	1.52	3 (17%)	20,30,33	3.17	7 (35%)
1	2MA	2A	2503	57,1	17,25,26	1.28	2 (11%)	19,37,40	1.89	3 (15%)
54	PSU	1w	39	54	17,21,22	1.45	2 (11%)	20,30,33	2.94	6 (30%)
32	2MG	2a	1207	32	19,26,27	1.27	2 (10%)	21,38,41	2.08	6 (28%)
56	PSU	1y	55	56	17,21,22	1.49	3 (17%)	20,30,33	3.06	5 (25%)
32	MA6	2a	1519	32	19,26,27	0.79	0	18,38,41	1.48	2 (11%)
32	M2G	2a	966	32	20,27,28	1.44	3 (15%)	22,40,43	2.14	6 (27%)
32	5MC	1a	1407	32	15,22,23	1.31	1 (6%)	19,32,35	1.29	3 (15%)
32	UR3	2a	1498	32	14,22,23	0.85	1 (7%)	15,32,35	0.85	1 (6%)
55	5MU	1x	54	55	15,22,23	1.07	1 (6%)	16,32,35	2.12	1 (6%)
56	4SU	2y	8	56	14,21,22	1.25	1 (7%)	15,30,33	1.51	2 (13%)
54	PSU	1w	55	54	17,21,22	1.42	2 (11%)	20,30,33	3.35	6 (30%)
54	MIA	1w	37	54	24,31,32	2.16	3 (12%)	26,44,47	2.58	9 (34%)
32	5MC	2a	1404	32	15,22,23	1.33	1 (6%)	19,32,35	1.37	3 (15%)
1	PSU	1A	1917	1	17,21,22	1.45	3 (17%)	20,30,33	3.08	6 (30%)
32	5MC	1a	1400	32	15,22,23	1.35	1 (6%)	19,32,35	1.30	3 (15%)
56	PSU	1y	32	56	17,21,22	1.42	2 (11%)	20,30,33	3.16	6 (30%)
54	PSU	1w	32	57,54	17,21,22	1.48	2 (11%)	20,30,33	3.20	6 (30%)
32	7MG	2a	527	32,57	22,26,27	1.81	4 (18%)	28,39,42	2.68	10 (35%)
56	7MG	2y	46	56	22,26,27	1.88	4 (18%)	28,39,42	2.98	10 (35%)
32	UR3	1a	1498	32	14,22,23	0.75	0	15,32,35	0.71	0
32	MA6	1a	1519	32	19,26,27	0.84	0	18,38,41	1.57	2 (11%)
54	PSU	2w	32	54	17,21,22	1.51	2 (11%)	20,30,33	3.16	6 (30%)
32	5MC	1a	1404	32	15,22,23	1.38	1 (6%)	19,32,35	1.24	3 (15%)
1	5MC	2A	1962	1	15,22,23	1.31	1 (6%)	19,32,35	1.31	3 (15%)
32	5MC	2a	967	32	15,22,23	1.33	1 (6%)	19,32,35	1.29	3 (15%)
56	MIA	1y	37	56	18,24,32	1.13	2 (11%)	18,35,47	1.30	2 (11%)
55	5MC	2x	32	55	15,22,23	1.28	1 (6%)	19,32,35	1.40	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMG	1A	2251	57,1,55	18,26,27	1.19	2 (11%)	20,38,41	2.17	5 (25%)
1	5MC	1A	1942	57,1	15,22,23	1.14	1 (6%)	19,32,35	1.67	4 (21%)
1	5MC	1A	1962	57,1	15,22,23	1.32	1 (6%)	19,32,35	1.34	2 (10%)
56	MIA	2y	37	56	18,24,32	1.11	2 (11%)	18,35,47	1.42	3 (16%)
54	7MG	1w	46	54	22,26,27	1.83	4 (18%)	28,39,42	2.72	8 (28%)
1	PSU	1A	2605	57,1	17,21,22	1.66	4 (23%)	20,30,33	3.18	6 (30%)
54	PSU	2w	55	54	17,21,22	1.45	2 (11%)	20,30,33	3.37	6 (30%)
1	OMC	1A	1920	1	15,22,23	0.71	0	17,31,34	1.49	2 (11%)
54	7MG	2w	46	54	22,26,27	1.80	4 (18%)	28,39,42	2.57	9 (32%)
55	4SU	2x	8	55	14,21,22	1.28	2 (14%)	15,30,33	2.39	2 (13%)
1	5MC	2A	1942	1	15,22,23	1.33	1 (6%)	19,32,35	1.48	3 (15%)
1	5MU	1A	1915	1	15,22,23	1.05	1 (6%)	16,32,35	1.69	2 (12%)
1	PSU	1A	1911	1	17,21,22	1.62	3 (17%)	20,30,33	2.97	6 (30%)
1	5MU	2A	1939	57,1	15,22,23	1.11	2 (13%)	16,32,35	1.80	2 (12%)
32	PSU	1a	516	32	17,21,22	1.43	3 (17%)	20,30,33	3.07	6 (30%)
56	PSU	2y	55	56	17,21,22	1.56	3 (17%)	20,30,33	3.14	6 (30%)
1	2MA	1A	2503	57,1	17,25,26	1.41	2 (11%)	19,37,40	1.97	3 (15%)
32	5MC	2a	1400	32	15,22,23	1.34	1 (6%)	19,32,35	1.32	3 (15%)
1	PSU	2A	1917	1	17,21,22	1.59	2 (11%)	20,30,33	3.15	6 (30%)
1	OMC	2A	1920	1	15,22,23	0.65	0	17,31,34	1.48	2 (11%)
43	0TD	1l	92	43	4,9,10	3.13	1 (25%)	3,11,13	7.23	1 (33%)
1	5MU	1A	1939	1	15,22,23	1.21	2 (13%)	16,32,35	2.00	2 (12%)
54	PSU	2w	39	54	17,21,22	1.49	3 (17%)	20,30,33	3.17	5 (25%)
55	5MU	2x	54	55	15,22,23	1.11	1 (6%)	16,32,35	1.78	2 (12%)
32	2MG	1a	1207	32	19,26,27	1.29	2 (10%)	21,38,41	2.38	7 (33%)
55	31H	1x	76	57,55	28,34,35	1.03	3 (10%)	23,47,50	1.57	3 (13%)
54	4SU	2w	8	54	14,21,22	1.24	1 (7%)	15,30,33	1.44	2 (13%)
32	7MG	1a	527	32,57	22,26,27	1.77	4 (18%)	28,39,42	2.65	10 (35%)
1	PSU	2A	1911	1	17,21,22	1.54	4 (23%)	20,30,33	3.17	6 (30%)
1	OMG	2A	2251	1,55	18,26,27	1.14	2 (11%)	20,38,41	2.05	6 (30%)
54	MIA	2w	37	54	20,27,32	1.65	3 (15%)	22,39,47	1.82	7 (31%)
32	MA6	2a	1518	32	19,26,27	0.80	0	18,38,41	1.46	2 (11%)
54	5MU	2w	54	54	15,22,23	1.10	1 (6%)	16,32,35	2.23	1 (6%)
55	31H	2x	76	57,55	28,34,35	1.04	3 (10%)	23,47,50	1.57	4 (17%)
56	7MG	1y	46	56	22,26,27	1.80	3 (13%)	28,39,42	2.84	9 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	M2G	1a	966	32	20,27,28	1.33	3 (15%)	22,40,43	2.25	7 (31%)
56	PSU	1y	39	56	17,21,22	1.39	2 (11%)	20,30,33	3.18	5 (25%)
56	5MU	1y	54	56	15,22,23	1.03	1 (6%)	16,32,35	2.42	1 (6%)
56	5MU	2y	54	56	15,22,23	1.06	1 (6%)	16,32,35	2.03	1 (6%)
1	5MU	2A	1915	1	15,22,23	1.09	1 (6%)	16,32,35	1.85	2 (12%)
32	4OC	2a	1402	32,57	16,23,24	0.63	0	17,32,35	1.58	1 (5%)
54	5MU	1w	54	54	15,22,23	1.08	1 (6%)	16,32,35	1.92	2 (12%)
55	5MC	1x	32	55	15,22,23	1.43	1 (6%)	19,32,35	1.30	3 (15%)
55	4SU	1x	8	55	14,21,22	1.36	2 (14%)	15,30,33	2.72	2 (13%)
43	0TD	2l	92	43	4,9,10	3.11	1 (25%)	3,11,13	5.94	1 (33%)
55	PSU	2x	55	55	17,21,22	1.61	2 (11%)	20,30,33	3.05	6 (30%)
55	PSU	1x	55	55	17,21,22	1.70	3 (17%)	20,30,33	3.11	6 (30%)
32	MA6	1a	1518	32	19,26,27	0.80	0	18,38,41	1.43	2 (11%)
1	PSU	2A	2605	1	17,21,22	1.49	3 (17%)	20,30,33	3.10	6 (30%)
56	PSU	2y	32	56	17,21,22	1.39	2 (11%)	20,30,33	3.05	5 (25%)
1	OMU	2A	2552	57,1	14,22,23	0.88	0	14,31,34	0.98	1 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	5MC	2a	1407	32	-	0/5/25/26	0/2/2/2
32	5MC	1a	967	32	-	0/5/25/26	0/2/2/2
56	PSU	2y	39	56	-	0/7/25/26	0/2/2/2
54	4SU	1w	8	54	-	0/5/25/26	0/2/2/2
32	4OC	1a	1402	32	-	0/9/29/30	0/2/2/2
1	OMU	1A	2552	57,1	-	0/7/27/28	0/2/2/2
56	4SU	1y	8	56	-	3/5/25/26	0/2/2/2
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	57,1	-	1/3/25/26	0/3/3/3
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	4/5/27/28	0/3/3/3
56	PSU	1y	55	56	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	3/7/29/30	0/3/3/3
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
32	5MC	1a	1407	32	-	0/5/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	UR3	2a	1498	32	-	0/5/25/26	0/2/2/2
55	5MU	1x	54	55	-	0/5/25/26	0/2/2/2
56	4SU	2y	8	56	-	0/5/25/26	0/2/2/2
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
54	MIA	1w	37	54	-	4/11/33/34	0/3/3/3
32	5MC	2a	1404	32	-	0/5/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	2/5/25/26	0/2/2/2
56	PSU	1y	32	56	-	0/7/25/26	0/2/2/2
54	PSU	1w	32	57,54	-	0/7/25/26	0/2/2/2
32	7MG	2a	527	32,57	-	3/7/37/38	0/3/3/3
56	7MG	2y	46	56	-	3/7/37/38	0/3/3/3
32	UR3	1a	1498	32	-	0/5/25/26	0/2/2/2
32	MA6	1a	1519	32	-	3/7/29/30	0/3/3/3
54	PSU	2w	32	54	-	2/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/5/25/26	0/2/2/2
1	5MC	2A	1962	1	-	2/5/25/26	0/2/2/2
32	5MC	2a	967	32	-	0/5/25/26	0/2/2/2
56	MIA	1y	37	56	-	0/3/25/34	0/3/3/3
55	5MC	2x	32	55	-	0/5/25/26	0/2/2/2
1	OMG	1A	2251	57,1,55	-	0/5/27/28	0/3/3/3
1	5MC	1A	1942	57,1	-	0/5/25/26	0/2/2/2
1	5MC	1A	1962	57,1	-	2/5/25/26	0/2/2/2
56	MIA	2y	37	56	-	0/3/25/34	0/3/3/3
54	7MG	1w	46	54	-	3/7/37/38	0/3/3/3
1	PSU	1A	2605	57,1	-	0/7/25/26	0/2/2/2
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
1	OMC	1A	1920	1	-	1/7/27/28	0/2/2/2
54	7MG	2w	46	54	-	1/7/37/38	0/3/3/3
55	4SU	2x	8	55	-	1/5/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/5/25/26	0/2/2/2
1	5MU	1A	1915	1	-	0/5/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	57,1	-	0/5/25/26	0/2/2/2
32	PSU	1a	516	32	-	0/7/25/26	0/2/2/2
56	PSU	2y	55	56	-	3/7/25/26	0/2/2/2
1	2MA	1A	2503	57,1	-	2/3/25/26	0/3/3/3
32	5MC	2a	1400	32	-	2/5/25/26	0/2/2/2
1	PSU	2A	1917	1	-	1/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMC	2A	1920	1	-	0/7/27/28	0/2/2/2
43	0TD	1l	92	43	-	2/3/12/14	-
1	5MU	1A	1939	1	-	0/5/25/26	0/2/2/2
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/5/25/26	0/2/2/2
32	2MG	1a	1207	32	-	0/5/27/28	0/3/3/3
55	31H	1x	76	57,55	-	4/18/40/41	0/3/3/3
54	4SU	2w	8	54	-	0/5/25/26	0/2/2/2
32	7MG	1a	527	32,57	-	3/7/37/38	0/3/3/3
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	1,55	-	0/5/27/28	0/3/3/3
54	MIA	2w	37	54	-	0/7/29/34	0/3/3/3
32	MA6	2a	1518	32	-	0/7/29/30	0/3/3/3
54	5MU	2w	54	54	-	0/5/25/26	0/2/2/2
55	31H	2x	76	57,55	-	3/18/40/41	0/3/3/3
56	7MG	1y	46	56	-	5/7/37/38	0/3/3/3
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
56	PSU	1y	39	56	-	0/7/25/26	0/2/2/2
56	5MU	1y	54	56	-	2/5/25/26	0/2/2/2
56	5MU	2y	54	56	-	3/5/25/26	0/2/2/2
1	5MU	2A	1915	1	-	0/5/25/26	0/2/2/2
32	4OC	2a	1402	32,57	-	4/9/29/30	0/2/2/2
54	5MU	1w	54	54	-	0/5/25/26	0/2/2/2
55	5MC	1x	32	55	-	0/5/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/5/25/26	0/2/2/2
43	0TD	2l	92	43	-	3/3/12/14	-
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/7/29/30	0/3/3/3
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
56	PSU	2y	32	56	-	0/7/25/26	0/2/2/2
1	OMU	2A	2552	57,1	-	0/7/27/28	0/2/2/2

All (152) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	37	MIA	C13-C14	7.18	1.53	1.32
54	1w	37	MIA	C2-S10	-6.20	1.70	1.75
43	2l	92	0TD	CB-SB	-5.99	1.69	1.84
43	1l	92	0TD	CB-SB	-5.90	1.69	1.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2w	37	MIA	C2-S10	-5.64	1.70	1.75
32	2a	527	7MG	C6-C5	5.42	1.48	1.41
55	1x	32	5MC	C5-C4	5.12	1.49	1.41
56	2y	46	7MG	C6-C5	5.08	1.48	1.41
54	2w	46	7MG	C6-C5	5.08	1.48	1.41
54	1w	46	7MG	C6-C5	4.94	1.48	1.41
32	1a	1404	5MC	C5-C4	4.90	1.48	1.41
55	1x	55	PSU	C5-C1'	-4.88	1.48	1.52
32	2a	967	5MC	C5-C4	4.85	1.48	1.41
56	1y	46	7MG	C6-C5	4.81	1.48	1.41
56	2y	46	7MG	C5-C4	4.80	1.48	1.39
1	2A	1942	5MC	C5-C4	4.78	1.48	1.41
32	2a	1407	5MC	C5-C4	4.75	1.48	1.41
32	1a	1400	5MC	C5-C4	4.75	1.48	1.41
32	2a	1400	5MC	C5-C4	4.74	1.48	1.41
32	2a	1404	5MC	C5-C4	4.73	1.48	1.41
1	2A	1962	5MC	C5-C4	4.70	1.48	1.41
32	1a	1207	2MG	C6-C5	4.69	1.49	1.41
1	1A	1962	5MC	C5-C4	4.69	1.48	1.41
54	1w	46	7MG	C5-C4	4.68	1.48	1.39
1	1A	2503	2MA	C6-C5	4.65	1.48	1.41
56	1y	46	7MG	C5-C4	4.64	1.48	1.39
32	1a	527	7MG	C6-C5	4.64	1.47	1.41
1	1A	2605	PSU	C5-C1'	-4.62	1.48	1.52
32	1a	967	5MC	C5-C4	4.61	1.48	1.41
55	2x	32	5MC	C5-C4	4.56	1.48	1.41
32	1a	1407	5MC	C5-C4	4.54	1.48	1.41
32	1a	527	7MG	C5-C4	4.51	1.48	1.39
55	2x	55	PSU	C5-C1'	-4.48	1.48	1.52
1	1A	1911	PSU	C5-C1'	-4.45	1.48	1.52
32	2a	1207	2MG	C6-C5	4.40	1.48	1.41
54	2w	46	7MG	C5-C4	4.39	1.47	1.39
32	2a	527	7MG	C5-C4	4.38	1.47	1.39
32	2a	966	M2G	C6-C5	4.32	1.48	1.41
1	2A	1917	PSU	C5-C1'	-4.28	1.48	1.52
56	2y	39	PSU	C5-C1'	-4.15	1.48	1.52
56	2y	55	PSU	C5-C1'	-4.14	1.48	1.52
1	2A	1911	PSU	C5-C1'	-4.12	1.48	1.52
1	2A	2503	2MA	C6-C5	4.12	1.47	1.41
32	1a	966	M2G	C6-C5	4.10	1.48	1.41
1	1A	1942	5MC	C5-C4	4.08	1.47	1.41
56	1y	8	4SU	C4-S4	-4.06	1.60	1.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	8	4SU	C4-S4	-4.00	1.60	1.67
32	2a	516	PSU	C5-C1'	-3.97	1.48	1.52
56	2y	8	4SU	C4-S4	-3.85	1.60	1.67
54	2w	39	PSU	C5-C1'	-3.84	1.49	1.52
54	2w	32	PSU	C5-C1'	-3.82	1.49	1.52
1	2A	2605	PSU	C5-C1'	-3.81	1.49	1.52
1	2A	2251	OMG	C6-C5	3.77	1.47	1.41
56	1y	55	PSU	C5-C1'	-3.73	1.49	1.52
54	2w	8	4SU	C4-S4	-3.71	1.60	1.67
1	1A	2251	OMG	C6-C5	3.67	1.47	1.41
54	2w	32	PSU	C4-C5	3.63	1.49	1.41
54	1w	32	PSU	C5-C1'	-3.61	1.49	1.52
55	2x	55	PSU	C4-C5	3.61	1.49	1.41
54	2w	55	PSU	C5-C1'	-3.59	1.49	1.52
56	1y	39	PSU	C4-C5	3.58	1.49	1.41
55	2x	8	4SU	C4-S4	-3.57	1.61	1.67
55	2x	54	5MU	C4-C5	3.55	1.49	1.41
56	1y	32	PSU	C4-C5	3.52	1.49	1.41
1	2A	1915	5MU	C4-C5	3.52	1.49	1.41
54	1w	39	PSU	C5-C1'	-3.51	1.49	1.52
55	1x	8	4SU	C4-S4	-3.51	1.61	1.67
56	2y	39	PSU	C4-C5	3.50	1.49	1.41
56	1y	46	7MG	C5-N7	-3.50	1.33	1.39
56	2y	55	PSU	C4-C5	3.49	1.49	1.41
1	2A	1917	PSU	C4-C5	3.48	1.48	1.41
54	1w	39	PSU	C4-C5	3.47	1.48	1.41
54	1w	32	PSU	C4-C5	3.47	1.48	1.41
1	1A	1917	PSU	C5-C1'	-3.46	1.49	1.52
32	1a	516	PSU	C4-C5	3.45	1.48	1.41
56	2y	32	PSU	C4-C5	3.44	1.48	1.41
54	2w	55	PSU	C4-C5	3.44	1.48	1.41
32	1a	527	7MG	C5-N7	-3.44	1.33	1.39
54	2w	54	5MU	C4-C5	3.41	1.48	1.41
56	1y	55	PSU	C4-C5	3.41	1.48	1.41
32	2a	516	PSU	C4-C5	3.40	1.48	1.41
56	2y	54	5MU	C4-C5	3.38	1.48	1.41
1	1A	1911	PSU	C4-C5	3.37	1.48	1.41
54	1w	54	5MU	C4-C5	3.36	1.48	1.41
32	2a	966	M2G	C2-N2	3.35	1.40	1.34
55	1x	55	PSU	C4-C5	3.33	1.48	1.41
56	1y	32	PSU	C5-C1'	-3.32	1.49	1.52
56	1y	54	5MU	C4-C5	3.31	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	55	PSU	C4-C5	3.31	1.48	1.41
54	1w	55	PSU	C5-C1'	-3.31	1.49	1.52
56	2y	46	7MG	C5-N7	-3.31	1.34	1.39
1	1A	1915	5MU	C4-C5	3.29	1.48	1.41
1	1A	1939	5MU	C4-C5	3.28	1.48	1.41
54	2w	39	PSU	C4-C5	3.28	1.48	1.41
55	1x	8	4SU	C2-N3	-3.26	1.31	1.38
55	1x	54	5MU	C4-C5	3.25	1.48	1.41
54	1w	46	7MG	C5-N7	-3.25	1.34	1.39
1	1A	1917	PSU	C4-C5	3.22	1.48	1.41
1	2A	2605	PSU	C4-C5	3.19	1.48	1.41
1	2A	1939	5MU	C4-C5	3.14	1.48	1.41
56	2y	32	PSU	C5-C1'	-3.13	1.49	1.52
32	2a	527	7MG	C5-N7	-3.11	1.34	1.39
1	2A	1911	PSU	C4-C5	3.10	1.48	1.41
32	1a	966	M2G	C2-N2	3.06	1.39	1.34
32	1a	516	PSU	C5-C1'	-3.04	1.49	1.52
1	1A	2605	PSU	C4-C5	3.01	1.47	1.41
54	2w	46	7MG	C5-N7	-3.00	1.34	1.39
55	2x	76	31H	C5-C4	-2.93	1.33	1.40
54	2w	46	7MG	C4-N9	-2.86	1.33	1.38
32	1a	527	7MG	C4-N9	-2.84	1.33	1.38
56	1y	39	PSU	C5-C1'	-2.82	1.49	1.52
55	1x	76	31H	C5-C4	-2.82	1.33	1.40
55	2x	8	4SU	C2-N3	-2.81	1.32	1.38
56	1y	37	MIA	C5-C4	2.72	1.48	1.40
54	2w	37	MIA	C5-C4	2.68	1.48	1.40
1	1A	1939	5MU	C2-N3	-2.68	1.32	1.38
32	2a	966	M2G	C5-C4	2.67	1.48	1.40
54	1w	46	7MG	C4-N9	-2.66	1.33	1.38
56	2y	37	MIA	C5-C4	2.65	1.47	1.40
56	2y	37	MIA	C2-N3	2.62	1.36	1.32
56	1y	37	MIA	C2-N3	2.61	1.36	1.32
32	2a	1207	2MG	C5-C4	2.60	1.47	1.40
55	1x	76	31H	C6-C5	-2.56	1.33	1.43
54	1w	37	MIA	C5-C4	2.56	1.47	1.40
1	1A	2251	OMG	C5-C4	2.55	1.47	1.40
32	1a	966	M2G	C5-C4	2.44	1.47	1.40
55	2x	76	31H	C6-C5	-2.43	1.34	1.43
1	2A	1939	5MU	C2-N3	-2.43	1.33	1.38
1	2A	2251	OMG	C5-C4	2.38	1.47	1.40
1	1A	2503	2MA	C5-C4	2.35	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2605	PSU	C2-N3	-2.28	1.33	1.38
32	1a	1207	2MG	C5-C4	2.27	1.46	1.40
32	2a	1498	UR3	C4-N3	2.24	1.41	1.38
56	2y	46	7MG	C4-N3	2.24	1.37	1.34
32	1a	516	PSU	O4'-C1'	-2.23	1.41	1.44
32	2a	527	7MG	C4-N9	-2.23	1.34	1.38
1	2A	2503	2MA	C5-C4	2.20	1.46	1.40
54	2w	37	MIA	C6-N1	2.18	1.35	1.32
1	1A	2605	PSU	C2-N1	-2.14	1.33	1.38
32	2a	516	PSU	O4'-C1'	-2.13	1.41	1.44
56	1y	8	4SU	C2-N3	-2.11	1.34	1.38
55	1x	76	31H	C5-N7	-2.09	1.32	1.39
55	2x	76	31H	C5-N7	-2.09	1.32	1.39
1	2A	1911	PSU	O4'-C1'	-2.09	1.41	1.44
55	1x	55	PSU	O4'-C1'	-2.09	1.41	1.44
1	1A	1917	PSU	C2-N3	-2.08	1.34	1.38
56	2y	55	PSU	C2-N1	-2.08	1.34	1.38
1	2A	2605	PSU	C2-N3	-2.07	1.34	1.38
56	1y	55	PSU	O4'-C1'	-2.07	1.41	1.44
54	2w	39	PSU	O4'-C1'	-2.07	1.41	1.44
1	1A	1911	PSU	O4'-C1'	-2.06	1.41	1.44
1	2A	1911	PSU	C2-N1	-2.04	1.34	1.38

All (342) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1l	92	0TD	CSB-SB-CB	-12.44	77.39	101.85
43	2l	92	0TD	CSB-SB-CB	-10.23	81.74	101.85
56	2y	46	7MG	N3-C4-N9	9.70	139.37	126.91
56	1y	46	7MG	N3-C4-N9	9.44	139.03	126.91
56	1y	54	5MU	C4-N3-C2	9.28	122.98	115.14
55	1x	8	4SU	C2-N3-C4	9.10	128.35	115.15
56	2y	39	PSU	N1-C2-N3	-9.01	121.27	128.43
54	2w	39	PSU	N1-C2-N3	-8.82	121.42	128.43
56	1y	39	PSU	N1-C2-N3	-8.78	121.45	128.43
1	2A	2605	PSU	N1-C2-N3	-8.78	121.45	128.43
32	2a	527	7MG	N3-C4-N9	8.77	138.18	126.91
32	1a	527	7MG	N3-C4-N9	8.70	138.08	126.91
54	1w	32	PSU	N1-C2-N3	-8.69	121.52	128.43
54	1w	46	7MG	N3-C4-N9	8.68	138.06	126.91
1	2A	1911	PSU	N1-C2-N3	-8.68	121.53	128.43
54	1w	55	PSU	N1-C2-N3	-8.67	121.54	128.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2w	32	PSU	N1-C2-N3	-8.64	121.56	128.43
54	2w	55	PSU	N1-C2-N3	-8.62	121.58	128.43
32	2a	516	PSU	N1-C2-N3	-8.57	121.62	128.43
56	1y	32	PSU	N1-C2-N3	-8.52	121.66	128.43
1	1A	1917	PSU	N1-C2-N3	-8.51	121.67	128.43
56	2y	55	PSU	N1-C2-N3	-8.48	121.69	128.43
54	2w	54	5MU	C4-N3-C2	8.48	122.30	115.14
32	1a	516	PSU	N1-C2-N3	-8.41	121.74	128.43
56	1y	55	PSU	N1-C2-N3	-8.41	121.75	128.43
56	2y	32	PSU	N1-C2-N3	-8.35	121.79	128.43
54	1w	39	PSU	N1-C2-N3	-8.18	121.92	128.43
1	1A	2605	PSU	N1-C2-N3	-8.18	121.93	128.43
54	1w	37	MIA	C12-C13-C14	-8.16	111.27	127.14
55	1x	54	5MU	C4-N3-C2	8.06	121.94	115.14
55	2x	55	PSU	N1-C2-N3	-7.89	122.16	128.43
55	2x	8	4SU	C2-N3-C4	7.86	126.55	115.15
54	2w	46	7MG	N3-C4-N9	7.79	136.92	126.91
55	1x	55	PSU	N1-C2-N3	-7.74	122.28	128.43
1	2A	1917	PSU	N1-C2-N3	-7.65	122.35	128.43
54	1w	55	PSU	C4-N3-C2	7.62	121.58	115.14
1	1A	1911	PSU	N1-C2-N3	-7.58	122.40	128.43
56	1y	39	PSU	C4-N3-C2	7.57	121.53	115.14
56	2y	54	5MU	C4-N3-C2	7.51	121.48	115.14
1	2A	1911	PSU	C4-N3-C2	7.36	121.35	115.14
54	1w	32	PSU	C4-N3-C2	7.35	121.34	115.14
54	2w	39	PSU	C4-N3-C2	7.27	121.28	115.14
54	1w	54	5MU	C4-N3-C2	7.12	121.16	115.14
32	1a	516	PSU	C4-N3-C2	7.11	121.14	115.14
56	2y	39	PSU	C4-N3-C2	7.11	121.14	115.14
56	2y	55	PSU	C4-N3-C2	7.07	121.11	115.14
32	2a	516	PSU	C4-N3-C2	7.05	121.09	115.14
1	1A	2605	PSU	C4-N3-C2	7.03	121.07	115.14
54	2w	32	PSU	C4-N3-C2	6.96	121.02	115.14
56	1y	55	PSU	C4-N3-C2	6.95	121.01	115.14
56	2y	32	PSU	C4-N3-C2	6.87	120.94	115.14
54	2w	55	PSU	C4-N3-C2	6.83	120.91	115.14
1	1A	1939	5MU	C4-N3-C2	6.78	120.87	115.14
56	1y	32	PSU	C4-N3-C2	6.72	120.81	115.14
1	2A	1915	5MU	C4-N3-C2	6.68	120.78	115.14
1	2A	1917	PSU	C4-N3-C2	6.67	120.77	115.14
55	1x	55	PSU	C4-N3-C2	6.61	120.72	115.14
1	1A	1917	PSU	C4-N3-C2	6.58	120.69	115.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	2x	55	PSU	C4-N3-C2	6.53	120.65	115.14
1	1A	1911	PSU	C4-N3-C2	6.33	120.49	115.14
1	2A	2605	PSU	C4-N3-C2	6.27	120.44	115.14
55	2x	54	5MU	C4-N3-C2	6.24	120.41	115.14
55	1x	55	PSU	C5-C4-N3	-6.13	117.46	125.36
1	1A	1915	5MU	C4-N3-C2	6.13	120.31	115.14
55	2x	76	31H	N3-C2-N1	-5.88	119.49	128.68
56	2y	55	PSU	C5-C4-N3	-5.82	117.87	125.36
1	2A	2503	2MA	C2-N3-C4	5.80	120.23	115.52
54	2w	55	PSU	C5-C1'-C2'	-5.78	105.00	115.32
54	2w	46	7MG	N7-C8-N9	-5.71	95.21	103.38
54	1w	39	PSU	C4-N3-C2	5.70	119.95	115.14
1	2A	1939	5MU	C4-N3-C2	5.70	119.95	115.14
1	2A	1917	PSU	C5-C4-N3	-5.64	118.09	125.36
1	1A	2503	2MA	C2-N3-C4	5.63	120.10	115.52
55	1x	76	31H	N3-C2-N1	-5.63	119.88	128.68
55	2x	55	PSU	C5-C4-N3	-5.62	118.12	125.36
56	1y	55	PSU	C5-C4-N3	-5.57	118.18	125.36
32	2a	516	PSU	C5-C4-N3	-5.56	118.19	125.36
32	2a	527	7MG	N7-C8-N9	-5.52	95.48	103.38
54	1w	32	PSU	C5-C4-N3	-5.51	118.26	125.36
56	1y	39	PSU	C5-C4-N3	-5.48	118.30	125.36
1	2A	1911	PSU	C5-C4-N3	-5.48	118.30	125.36
54	1w	55	PSU	C5-C4-N3	-5.47	118.32	125.36
1	1A	2605	PSU	C5-C4-N3	-5.46	118.32	125.36
54	1w	46	7MG	N7-C8-N9	-5.40	95.66	103.38
54	2w	39	PSU	C5-C4-N3	-5.38	118.42	125.36
32	1a	516	PSU	C5-C4-N3	-5.35	118.46	125.36
56	1y	46	7MG	C5-C4-N3	-5.35	117.75	126.49
54	2w	32	PSU	C5-C4-N3	-5.35	118.47	125.36
56	2y	46	7MG	C5-C4-N3	-5.35	117.76	126.49
56	2y	39	PSU	C5-C4-N3	-5.34	118.48	125.36
1	1A	1911	PSU	C5-C4-N3	-5.30	118.53	125.36
56	2y	32	PSU	C5-C4-N3	-5.29	118.55	125.36
56	2y	46	7MG	C6-N1-C2	5.27	124.30	115.93
54	1w	55	PSU	C5-C1'-C2'	-5.23	106.00	115.32
54	2w	55	PSU	C5-C4-N3	-5.20	118.66	125.36
32	1a	966	M2G	C6-N1-C2	5.16	122.32	116.18
32	2a	1402	4OC	CM4-N4-C4	-5.16	118.54	122.97
32	1a	1207	2MG	C2-N3-C4	5.12	121.09	115.28
32	2a	966	M2G	C2-N3-C4	5.12	121.09	115.28
56	2y	46	7MG	N7-C8-N9	-5.09	96.10	103.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	1y	32	PSU	C5-C4-N3	-5.08	118.82	125.36
32	2a	1518	MA6	N3-C2-N1	-5.07	120.76	128.68
32	2a	527	7MG	C5-C4-N3	-5.03	118.27	126.49
1	1A	1917	PSU	C5-C4-N3	-4.99	118.93	125.36
1	1A	2503	2MA	C5-C6-N1	-4.96	117.86	123.06
32	1a	527	7MG	C5-C4-N3	-4.92	118.46	126.49
32	2a	966	M2G	C6-N1-C2	4.91	122.03	116.18
32	1a	1519	MA6	N3-C2-N1	-4.91	121.00	128.68
54	1w	39	PSU	C5-C4-N3	-4.90	119.04	125.36
32	1a	527	7MG	N7-C8-N9	-4.89	96.39	103.38
56	1y	46	7MG	N7-C8-N9	-4.88	96.39	103.38
55	1x	8	4SU	C5-C4-N3	-4.82	117.38	123.83
56	1y	46	7MG	C6-N1-C2	4.80	123.56	115.93
1	1A	2251	OMG	C2-N3-C4	4.78	120.82	115.36
32	2a	1519	MA6	N3-C2-N1	-4.77	121.23	128.68
54	2w	37	MIA	C2-N3-C4	4.73	121.84	115.32
32	1a	1518	MA6	N3-C2-N1	-4.71	121.32	128.68
54	1w	46	7MG	C6-N1-C2	4.68	123.37	115.93
1	2A	1920	OMC	C2-N3-C4	4.65	121.06	116.34
32	2a	1207	2MG	C2-N3-C4	4.65	120.56	115.28
54	2w	46	7MG	C6-N1-C2	4.62	123.28	115.93
1	2A	2605	PSU	C5-C4-N3	-4.62	119.41	125.36
32	1a	966	M2G	C2-N3-C4	4.62	120.52	115.28
54	1w	46	7MG	C5-C4-N3	-4.59	119.00	126.49
1	2A	2503	2MA	C5-C6-N1	-4.56	118.28	123.06
54	1w	8	4SU	C2-N3-C4	4.52	121.70	115.15
54	1w	37	MIA	C2-N3-C4	4.50	121.52	115.32
1	1A	1920	OMC	C2-N3-C4	4.45	120.85	116.34
55	2x	8	4SU	C5-C4-N3	-4.44	117.89	123.83
1	2A	1917	PSU	C5-C1'-C2'	-4.44	107.40	115.32
56	2y	8	4SU	C2-N3-C4	4.44	121.58	115.15
56	2y	39	PSU	C5-C1'-C2'	-4.42	107.43	115.32
1	2A	2251	OMG	C2-N3-C4	4.39	120.38	115.36
56	1y	46	7MG	C6-C5-C4	4.39	119.92	115.20
1	2A	1917	PSU	C5-C6-N1	-4.37	119.06	124.44
54	1w	37	MIA	C15-C14-C13	-4.36	110.05	122.65
1	1A	1911	PSU	C5-C6-N1	-4.34	119.10	124.44
32	1a	527	7MG	C6-N1-C2	4.33	122.81	115.93
56	2y	46	7MG	C6-C5-C4	4.33	119.84	115.20
1	2A	2605	PSU	C6-N1-C2	4.33	122.50	115.36
54	1w	39	PSU	C6-N1-C2	4.32	122.48	115.36
55	2x	55	PSU	C5-C6-N1	-4.30	119.15	124.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2251	OMG	C6-N1-C2	4.29	122.75	115.93
56	2y	39	PSU	C6-N1-C2	4.24	122.35	115.36
1	1A	2605	PSU	C5-C6-N1	-4.23	119.24	124.44
56	2y	39	PSU	C5-C6-N1	-4.23	119.25	124.44
1	1A	1962	5MC	C2-N3-C4	4.22	121.12	116.02
54	1w	39	PSU	C5-C6-N1	-4.22	119.26	124.44
54	2w	46	7MG	C5-C4-N3	-4.20	119.63	126.49
32	2a	527	7MG	C6-N1-C2	4.18	122.57	115.93
1	1A	1917	PSU	C6-N1-C2	4.17	122.25	115.36
1	2A	2605	PSU	C5-C6-N1	-4.15	119.33	124.44
32	2a	1207	2MG	C5-C6-N1	-4.15	117.75	123.43
54	2w	55	PSU	C6-N1-C2	4.15	122.20	115.36
56	1y	8	4SU	C2-N3-C4	4.12	121.13	115.15
32	1a	1207	2MG	C6-C5-C4	-4.11	116.88	120.80
56	1y	32	PSU	C6-N1-C2	4.10	122.12	115.36
32	1a	1207	2MG	C5-C6-N1	-4.09	117.84	123.43
54	2w	8	4SU	C2-N3-C4	4.06	121.03	115.15
56	1y	32	PSU	C5-C6-N1	-4.05	119.46	124.44
54	2w	32	PSU	C6-N1-C2	4.04	122.02	115.36
1	2A	2251	OMG	C6-N1-C2	4.03	122.33	115.93
54	2w	55	PSU	C5-C6-N1	-4.02	119.50	124.44
32	2a	516	PSU	C6-N1-C2	4.01	121.98	115.36
1	1A	1917	PSU	C5-C6-N1	-4.01	119.51	124.44
1	1A	2251	OMG	C6-C5-C4	-4.00	116.98	120.80
56	2y	55	PSU	C6-N1-C2	4.00	121.96	115.36
32	2a	966	M2G	C5-C6-N1	-4.00	117.96	123.43
32	2a	516	PSU	C5-C6-N1	-3.98	119.55	124.44
54	1w	46	7MG	C6-C5-C4	3.98	119.47	115.20
1	2A	2251	OMG	C5-C6-N1	-3.97	118.00	123.43
54	2w	39	PSU	C6-N1-C2	3.97	121.91	115.36
32	1a	527	7MG	C6-C5-C4	3.97	119.46	115.20
55	2x	55	PSU	C6-N1-C2	3.97	121.91	115.36
55	1x	55	PSU	C5-C6-N1	-3.96	119.58	124.44
1	1A	2605	PSU	C6-N1-C2	3.94	121.86	115.36
32	1a	516	PSU	C6-N1-C2	3.93	121.85	115.36
32	1a	966	M2G	C6-C5-C4	-3.93	117.05	120.80
56	2y	32	PSU	C6-N1-C2	3.93	121.84	115.36
54	2w	32	PSU	C5-C6-N1	-3.91	119.63	124.44
56	1y	39	PSU	C6-N1-C2	3.91	121.81	115.36
54	1w	32	PSU	C6-N1-C2	3.90	121.79	115.36
54	1w	46	7MG	C5-C6-N1	-3.88	115.16	123.14
32	1a	966	M2G	C5-C6-N1	-3.88	118.12	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	2y	32	PSU	C5-C6-N1	-3.87	119.68	124.44
32	1a	967	5MC	C2-N3-C4	3.87	120.69	116.02
1	1A	1911	PSU	C6-N1-C2	3.86	121.73	115.36
32	1a	516	PSU	C5-C6-N1	-3.86	119.70	124.44
32	2a	1207	2MG	C6-N1-C2	3.85	122.07	115.18
1	2A	1917	PSU	C6-N1-C2	3.84	121.70	115.36
54	2w	39	PSU	C5-C6-N1	-3.84	119.72	124.44
32	1a	1207	2MG	C4-C5-N7	-3.84	105.40	109.40
32	1a	1207	2MG	C6-N1-C2	3.83	122.04	115.18
1	2A	1911	PSU	C6-N1-C2	3.80	121.62	115.36
56	2y	46	7MG	C5-C6-N1	-3.78	115.37	123.14
1	1A	2251	OMG	N3-C2-N1	-3.77	122.20	127.22
56	1y	55	PSU	C6-N1-C2	3.76	121.56	115.36
55	2x	32	5MC	C2-N3-C4	3.75	120.55	116.02
54	1w	37	MIA	C16-C14-C13	-3.75	111.82	122.65
56	1y	46	7MG	C5-C6-N1	-3.73	115.48	123.14
32	2a	967	5MC	C2-N3-C4	3.73	120.52	116.02
55	1x	55	PSU	C6-N1-C2	3.73	121.50	115.36
56	2y	37	MIA	N3-C2-N1	-3.72	122.86	128.68
55	1x	55	PSU	C5-C1'-C2'	-3.72	108.69	115.32
1	1A	1942	5MC	C2-N3-C4	3.70	120.49	116.02
54	2w	46	7MG	C5-C6-N1	-3.67	115.60	123.14
1	1A	2251	OMG	C5-C6-N1	-3.67	118.42	123.43
54	1w	37	MIA	C12-N6-C6	-3.64	117.15	122.55
32	2a	1407	5MC	C2-N3-C4	3.64	120.41	116.02
32	2a	527	7MG	C6-C5-C4	3.63	119.10	115.20
56	1y	37	MIA	N3-C2-N1	-3.62	123.01	128.68
56	2y	55	PSU	C5-C6-N1	-3.62	119.99	124.44
1	2A	2251	OMG	C6-C5-C4	-3.62	117.35	120.80
56	1y	39	PSU	C5-C6-N1	-3.61	120.01	124.44
54	1w	55	PSU	C6-N1-C2	3.60	121.30	115.36
1	1A	1942	5MC	N4-C4-N3	3.60	122.12	117.03
32	1a	527	7MG	C5-C6-N1	-3.58	115.78	123.14
32	1a	966	M2G	CM2-N2-C2	-3.56	117.90	121.29
32	1a	1407	5MC	C2-N3-C4	3.55	120.30	116.02
32	1a	1404	5MC	C2-N3-C4	3.55	120.30	116.02
32	2a	1404	5MC	C2-N3-C4	3.53	120.28	116.02
32	1a	1400	5MC	C2-N3-C4	3.53	120.28	116.02
1	2A	1911	PSU	C5-C6-N1	-3.51	120.13	124.44
1	1A	2605	PSU	C5-C1'-C2'	-3.47	109.14	115.32
54	1w	32	PSU	C5-C6-N1	-3.46	120.18	124.44
32	2a	1400	5MC	C2-N3-C4	3.45	120.18	116.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	527	7MG	C5-C6-N1	-3.43	116.09	123.14
1	2A	1942	5MC	C2-N3-C4	3.42	120.14	116.02
1	2A	1939	5MU	C5-C6-N1	-3.40	118.53	122.19
32	1a	1207	2MG	CM2-N2-C2	-3.38	119.51	123.59
1	2A	1962	5MC	C2-N3-C4	3.37	120.08	116.02
32	2a	1207	2MG	C6-C5-C4	-3.36	117.59	120.80
55	1x	32	5MC	C2-N3-C4	3.32	120.02	116.02
56	1y	55	PSU	C5-C6-N1	-3.31	120.37	124.44
32	1a	1519	MA6	C4-C5-N7	-3.29	105.97	109.40
1	1A	1939	5MU	C5-C6-N1	-3.28	118.65	122.19
32	2a	1519	MA6	C4-C5-N7	-3.27	105.99	109.40
54	1w	37	MIA	C5-C6-N1	-3.23	118.13	120.81
1	2A	2251	OMG	N3-C2-N1	-3.22	122.93	127.22
56	1y	32	PSU	C5-C1'-C2'	-3.21	109.58	115.32
54	2w	37	MIA	C5-C6-N1	-3.21	118.14	120.81
54	2w	37	MIA	C12-N6-C6	-3.17	120.14	122.87
54	2w	46	7MG	C6-C5-C4	3.15	118.58	115.20
55	1x	76	31H	CA-N-CN	-3.12	118.02	122.82
54	2w	8	4SU	C5-C4-N3	-3.12	119.66	123.83
56	2y	8	4SU	C5-C4-N3	-3.10	119.68	123.83
32	1a	1518	MA6	C4-C5-N7	-3.04	106.23	109.40
1	1A	1911	PSU	C5-C1'-C2'	-3.03	109.92	115.32
1	2A	1962	5MC	N4-C4-N3	3.03	121.31	117.03
54	1w	37	MIA	C2-N1-C6	3.01	122.58	117.19
1	2A	2605	PSU	C5-C1'-C2'	-3.00	109.96	115.32
32	2a	966	M2G	C6-C5-C4	-3.00	117.94	120.80
32	1a	1207	2MG	N2-C2-N1	2.98	119.82	116.96
56	2y	37	MIA	C4-C5-N7	-2.95	106.32	109.40
54	1w	55	PSU	C5-C6-N1	-2.94	120.82	124.44
55	2x	32	5MC	N4-C4-N3	2.94	121.19	117.03
54	1w	8	4SU	C5-C4-N3	-2.93	119.91	123.83
1	1A	1942	5MC	CM5-C5-C4	-2.90	118.78	121.72
56	1y	8	4SU	C5-C4-N3	-2.90	119.95	123.83
55	1x	32	5MC	C5-C6-N1	-2.87	119.11	122.19
32	1a	966	M2G	N3-C2-N2	2.85	120.08	117.18
54	1w	32	PSU	C5-C1'-C2'	-2.85	110.24	115.32
32	2a	1207	2MG	C4-C5-N7	-2.84	106.44	109.40
1	2A	1942	5MC	N4-C4-N3	2.84	121.04	117.03
56	1y	37	MIA	C4-C5-N7	-2.83	106.45	109.40
32	2a	527	7MG	C8-N7-C5	2.83	116.29	108.94
55	2x	55	PSU	C5-C1'-C2'	-2.80	110.33	115.32
54	2w	32	PSU	C5-C1'-C2'	-2.78	110.35	115.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	2y	46	7MG	C8-N7-C5	2.76	116.12	108.94
32	2a	1518	MA6	C4-C5-N7	-2.75	106.53	109.40
54	1w	37	MIA	N3-C2-N1	-2.75	121.92	126.98
55	2x	54	5MU	C5-C6-N1	-2.73	119.25	122.19
1	1A	1917	PSU	C5-C1'-C2'	-2.69	110.52	115.32
32	2a	966	M2G	N3-C2-N2	2.69	119.91	117.18
54	2w	46	7MG	C8-N7-C5	2.66	115.87	108.94
32	1a	967	5MC	N4-C4-N3	2.66	120.79	117.03
1	1A	1942	5MC	C5-C6-N1	-2.65	119.33	122.19
1	2A	1942	5MC	C5-C6-N1	-2.64	119.35	122.19
32	2a	1400	5MC	C5-C6-N1	-2.63	119.36	122.19
32	2a	1498	UR3	C3U-N3-C4	2.63	121.60	118.12
54	2w	37	MIA	C4-C5-N7	-2.62	106.67	109.40
54	1w	46	7MG	C8-N7-C5	2.60	115.70	108.94
1	1A	1920	OMC	N4-C4-N3	2.59	120.59	116.49
54	1w	37	MIA	C4-C5-N7	-2.58	106.71	109.40
56	2y	46	7MG	C5-C4-N9	-2.58	102.83	106.44
54	2w	37	MIA	C2-N1-C6	2.57	121.78	117.19
32	1a	966	M2G	C4-C5-N7	-2.56	106.73	109.40
56	1y	46	7MG	C8-N7-C5	2.54	115.56	108.94
32	2a	1404	5MC	N4-C4-N3	2.52	120.59	117.03
32	2a	1407	5MC	C5-C6-N1	-2.52	119.48	122.19
54	1w	46	7MG	C5-C4-N9	-2.50	102.94	106.44
32	2a	1207	2MG	N2-C2-N3	2.50	119.36	116.96
32	1a	527	7MG	C8-N7-C5	2.47	115.35	108.94
54	2w	37	MIA	N3-C2-N1	-2.45	122.48	126.98
32	2a	516	PSU	C5-C1'-C2'	-2.44	110.96	115.32
55	2x	76	31H	CA-N-CN	-2.42	119.10	122.82
32	2a	1404	5MC	C5-C6-N1	-2.41	119.60	122.19
32	1a	1404	5MC	C5-C6-N1	-2.40	119.60	122.19
32	2a	1400	5MC	N4-C4-N3	2.40	120.43	117.03
32	1a	1400	5MC	C5-C6-N1	-2.40	119.61	122.19
1	2A	1915	5MU	C5-C6-N1	-2.39	119.62	122.19
32	2a	1407	5MC	N4-C4-N3	2.37	120.38	117.03
32	1a	1400	5MC	N4-C4-N3	2.36	120.37	117.03
54	1w	39	PSU	C5-C1'-C2'	-2.36	111.11	115.32
1	1A	2503	2MA	C4-C5-N7	-2.36	106.94	109.40
32	2a	516	PSU	O4'-C1'-C2'	2.32	108.42	104.66
56	1y	46	7MG	C5-C4-N9	-2.31	103.21	106.44
55	1x	32	5MC	N4-C4-N3	2.30	120.28	117.03
1	2A	2503	2MA	C4-C5-N7	-2.28	107.02	109.40
56	2y	46	7MG	C2-N3-C4	2.28	120.19	113.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	966	M2G	C4-C5-N7	-2.28	107.03	109.40
32	2a	967	5MC	N4-C4-N3	2.27	120.24	117.03
1	1A	2552	OMU	C5-C4-N3	-2.27	118.31	123.31
32	1a	527	7MG	CM7-N7-C5	2.25	132.67	124.01
1	1A	1915	5MU	C5-C6-N1	-2.23	119.79	122.19
32	2a	527	7MG	C2-N3-C4	2.22	120.03	113.89
32	1a	1404	5MC	N4-C4-N3	2.22	120.17	117.03
56	1y	46	7MG	C2-N3-C4	2.22	120.02	113.89
1	2A	1920	OMC	N4-C4-N3	2.22	119.99	116.49
56	2y	55	PSU	O4'-C1'-C2'	2.21	108.23	104.66
1	2A	2552	OMU	C5-C4-N3	-2.20	118.47	123.31
1	2A	1962	5MC	C5-C6-N1	-2.19	119.83	122.19
1	2A	2251	OMG	C4-C5-N7	-2.16	107.14	109.40
55	1x	76	31H	OCN-CN-N	-2.16	119.58	125.27
32	1a	1407	5MC	N4-C4-N3	2.16	120.09	117.03
32	2a	967	5MC	C5-C6-N1	-2.15	119.87	122.19
32	1a	527	7MG	C5-C4-N9	-2.15	103.44	106.44
56	2y	46	7MG	O4'-C1'-N9	-2.14	106.45	109.35
54	2w	46	7MG	C5-C4-N9	-2.14	103.45	106.44
32	1a	1407	5MC	C5-C6-N1	-2.12	119.92	122.19
32	1a	527	7MG	C2-N3-C4	2.10	119.69	113.89
32	1a	516	PSU	O4'-C1'-C2'	2.09	108.04	104.66
1	1A	1962	5MC	N4-C4-N3	2.08	119.97	117.03
54	1w	54	5MU	C5-C6-N1	-2.08	119.95	122.19
32	2a	527	7MG	C5-C4-N9	-2.08	103.53	106.44
54	2w	46	7MG	C2-N3-C4	2.04	119.53	113.89
32	2a	527	7MG	CM7-N7-C5	2.03	131.79	124.01
55	2x	76	31H	O4'-C1'-C2'	-2.02	103.97	106.93
54	2w	37	MIA	N6-C6-N1	2.01	121.01	118.50
56	2y	37	MIA	C2-N1-C6	2.01	122.19	118.75
1	2A	1911	PSU	C5-C1'-C2'	-2.00	111.74	115.32
55	2x	76	31H	OCN-CN-N	-2.00	119.99	125.27

There are no chirality outliers.

All (75) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
43	1l	92	0TD	CA-CB-SB-CSB
43	1l	92	0TD	CG-CB-SB-CSB
56	1y	46	7MG	C4'-C5'-O5'-P
43	2l	92	0TD	O-C-CA-CB
43	2l	92	0TD	CG-CB-SB-CSB

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Mol	Chain	Res	Type	Atoms
56	2y	54	5MU	C2'-C1'-N1-C6
56	2y	54	5MU	C3'-C4'-C5'-O5'
56	2y	54	5MU	O4'-C4'-C5'-O5'
56	2y	55	PSU	O4'-C1'-C5-C4
56	2y	55	PSU	C2'-C1'-C5-C6
56	2y	55	PSU	O4'-C1'-C5-C6
1	1A	1920	OMC	C2'-C1'-N1-C6
1	1A	1962	5MC	O4'-C1'-N1-C6
1	1A	1962	5MC	C2'-C1'-N1-C6
1	2A	1962	5MC	O4'-C1'-N1-C6
1	2A	1962	5MC	C2'-C1'-N1-C6
32	2a	1207	2MG	O4'-C4'-C5'-O5'
32	2a	1207	2MG	C3'-C4'-C5'-O5'
32	2a	1207	2MG	N1-C2-N2-CM2
32	2a	1207	2MG	N3-C2-N2-CM2
32	2a	1400	5MC	O4'-C1'-N1-C6
32	2a	1400	5MC	C2'-C1'-N1-C6
32	2a	1402	4OC	O4'-C1'-N1-C6
32	2a	1402	4OC	C2'-C1'-N1-C6
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
54	1w	37	MIA	C12-C13-C14-C16
55	2x	8	4SU	O4'-C1'-N1-C6
55	2x	76	31H	C3'-C4'-C5'-O5'
32	1a	527	7MG	C3'-C4'-C5'-O5'
32	2a	1402	4OC	O4'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
55	1x	76	31H	C3'-C4'-C5'-O5'
56	1y	8	4SU	C3'-C4'-C5'-O5'
56	1y	8	4SU	O4'-C4'-C5'-O5'
32	2a	1402	4OC	C3'-C4'-C5'-O5'
55	1x	76	31H	C4'-C5'-O5'-P
32	2a	527	7MG	C3'-C4'-C5'-O5'
56	1y	54	5MU	O4'-C4'-C5'-O5'
32	1a	527	7MG	O4'-C4'-C5'-O5'
32	1a	1400	5MC	O4'-C4'-C5'-O5'
55	1x	76	31H	O4'-C4'-C5'-O5'
55	2x	76	31H	O4'-C4'-C5'-O5'
54	2w	32	PSU	O4'-C4'-C5'-O5'
54	2w	46	7MG	C4'-C5'-O5'-P
32	2a	527	7MG	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
56	2y	46	7MG	O4'-C1'-N9-C4
56	2y	46	7MG	O4'-C1'-N9-C8
55	1x	76	31H	CA-CB-CG-SD
55	2x	76	31H	C4'-C5'-O5'-P
54	1w	46	7MG	C3'-C4'-C5'-O5'
32	1a	1519	MA6	C4'-C5'-O5'-P
56	1y	46	7MG	C2'-C1'-N9-C8
56	2y	46	7MG	C2'-C1'-N9-C8
32	1a	1400	5MC	C3'-C4'-C5'-O5'
54	1w	46	7MG	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C4'-C5'-O5'-P
54	1w	37	MIA	N1-C2-S10-C11
32	1a	527	7MG	C4'-C5'-O5'-P
54	1w	46	7MG	C4'-C5'-O5'-P
56	1y	46	7MG	C3'-C4'-C5'-O5'
1	2A	1917	PSU	O4'-C4'-C5'-O5'
1	1A	2503	2MA	O4'-C4'-C5'-O5'
54	1w	37	MIA	N3-C2-S10-C11
32	2a	527	7MG	C4'-C5'-O5'-P
1	2A	2503	2MA	O4'-C4'-C5'-O5'
54	1w	37	MIA	N6-C12-C13-C14
56	1y	46	7MG	O4'-C1'-N9-C8
43	2l	92	0TD	CA-CB-SB-CSB
56	1y	8	4SU	C4'-C5'-O5'-P
1	1A	2503	2MA	C4'-C5'-O5'-P
56	1y	54	5MU	C3'-C4'-C5'-O5'
54	2w	32	PSU	C3'-C4'-C5'-O5'
56	1y	46	7MG	C2'-C1'-N9-C4

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 2586 ligands modelled in this entry, 2582 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
60	SF4	1d	302	35	0,12,12	-	-	-	-	-
58	6IF	1A	4109	-	30,34,34	1.02	2 (6%)	32,49,49	1.71	4 (12%)
60	SF4	2d	302	35	0,12,12	-	-	-	-	-
58	6IF	2A	3731	-	30,34,34	0.80	1 (3%)	32,49,49	1.59	4 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	SF4	1d	302	35	-	-	0/6/5/5
58	6IF	1A	4109	-	-	4/22/65/65	0/3/3/3
60	SF4	2d	302	35	-	-	0/6/5/5
58	6IF	2A	3731	-	-	2/22/65/65	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	1A	4109	6IF	CG-CB	-2.37	1.49	1.53
58	2A	3731	6IF	CAI-CLAJ	-2.23	1.77	1.81
58	1A	4109	6IF	CAA-CAB	-2.02	1.49	1.53

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	1A	4109	6IF	CBB-CBA-CAY	-6.20	110.73	116.03
58	2A	3731	6IF	CBB-CBA-CAY	-5.45	111.37	116.03
58	2A	3731	6IF	CD1-CG-CB	-4.84	97.81	103.80
58	1A	4109	6IF	CD1-CG-CB	-4.73	97.95	103.80
58	1A	4109	6IF	CAK-CAI-CAG	-3.09	110.28	114.26
58	2A	3731	6IF	CD2-CAY-CAX	-2.58	110.03	113.89
58	2A	3731	6IF	CAK-CAI-CAG	-2.50	111.04	114.26
58	1A	4109	6IF	CD2-CAY-CAX	-2.10	110.74	113.89

There are no chirality outliers.

All (6) torsion outliers are listed below:

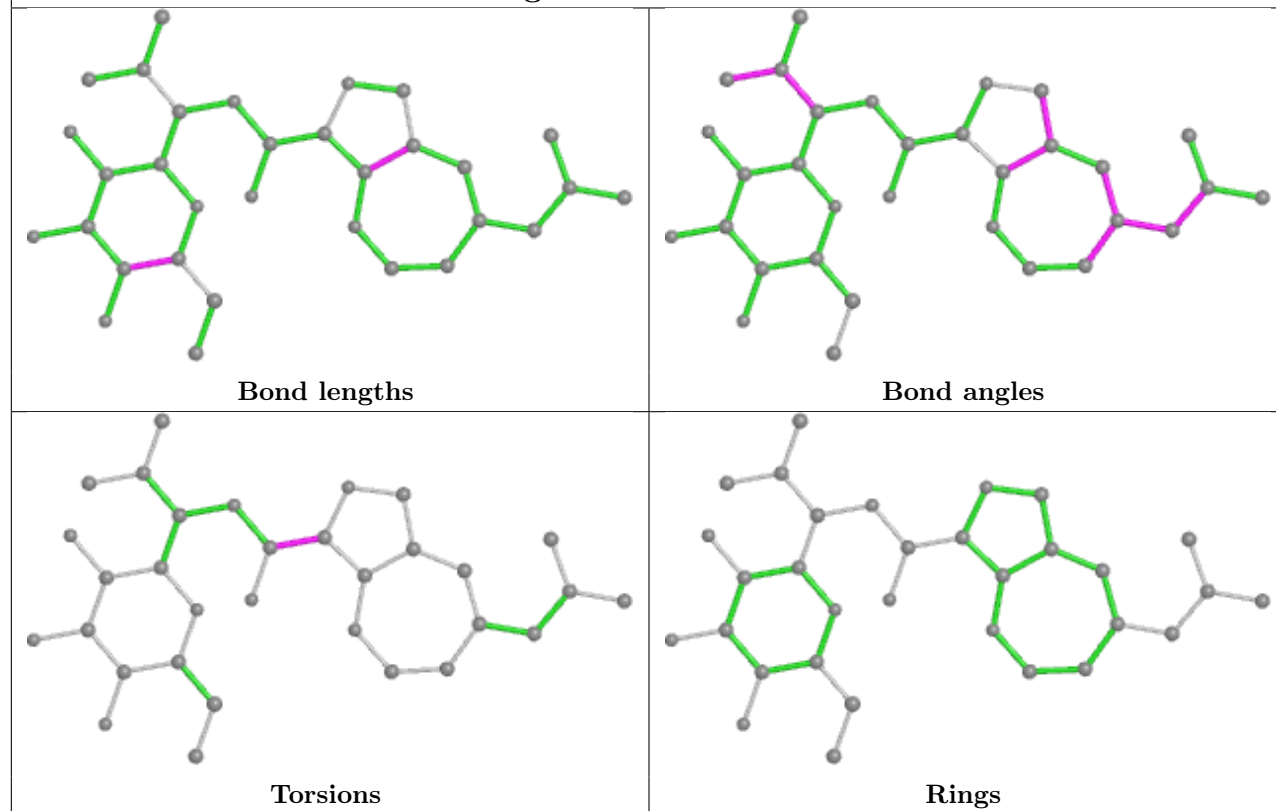
Mol	Chain	Res	Type	Atoms
58	1A	4109	6IF	O-C-CA-CB
58	1A	4109	6IF	NAH-C-CA-CB
58	2A	3731	6IF	NAH-C-CA-CB
58	1A	4109	6IF	NAH-C-CA-N
58	2A	3731	6IF	O-C-CA-CB
58	1A	4109	6IF	O-C-CA-N

There are no ring outliers.

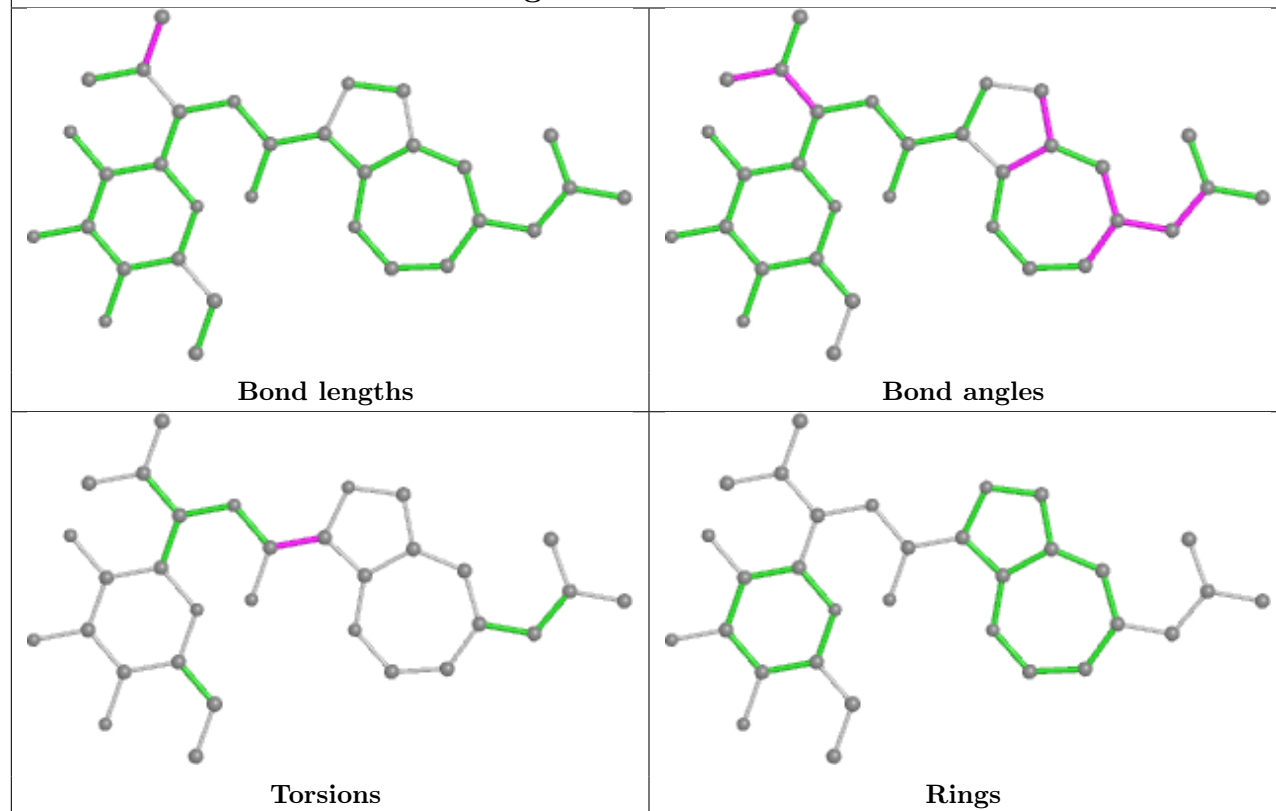
No monomer is involved in short contacts.

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

Ligand 6IF 1A 4109



Ligand 6IF 2A 3731



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1A	2860/2915 (98%)	0.42	68 (2%) 59 62	19, 36, 89, 102	0
1	2A	2789/2915 (95%)	0.17	80 (2%) 51 55	34, 57, 89, 99	0
2	1B	120/121 (99%)	0.20	0 100 100	29, 47, 62, 82	0
2	2B	120/121 (99%)	0.08	3 (2%) 57 61	62, 80, 88, 92	0
3	1D	275/276 (99%)	0.52	2 (0%) 87 89	21, 37, 51, 74	0
3	2D	275/276 (99%)	0.71	12 (4%) 34 37	33, 52, 64, 81	0
4	1E	204/206 (99%)	0.55	1 (0%) 91 91	18, 40, 58, 71	0
4	2E	204/206 (99%)	0.66	6 (2%) 51 55	33, 56, 68, 74	0
5	1F	203/210 (96%)	0.56	0 100 100	20, 41, 65, 79	0
5	2F	203/210 (96%)	0.42	4 (1%) 65 68	35, 66, 77, 83	0
6	1G	181/182 (99%)	0.31	4 (2%) 62 65	38, 56, 69, 83	0
6	2G	181/182 (99%)	1.09	36 (19%) 1 1	72, 79, 83, 88	0
7	1H	174/180 (96%)	0.36	0 100 100	36, 52, 63, 67	0
7	2H	174/180 (96%)	2.27	95 (54%) 0 0	66, 78, 85, 88	0
8	1I	146/148 (98%)	0.35	2 (1%) 75 77	45, 70, 79, 83	0
8	2I	146/148 (98%)	1.05	32 (21%) 0 0	53, 71, 79, 83	0
9	1N	140/140 (100%)	0.67	0 100 100	24, 39, 56, 71	0
9	2N	140/140 (100%)	0.75	13 (9%) 8 8	45, 63, 75, 79	0
10	1O	122/122 (100%)	0.49	1 (0%) 86 87	25, 40, 57, 62	0
10	2O	122/122 (100%)	0.81	9 (7%) 14 15	47, 57, 69, 73	0
11	1P	149/150 (99%)	0.55	2 (1%) 77 79	20, 44, 65, 71	0
11	2P	149/150 (99%)	0.83	12 (8%) 12 12	38, 65, 79, 83	0
12	1Q	141/141 (100%)	0.62	3 (2%) 63 66	28, 41, 56, 70	0
12	2Q	141/141 (100%)	1.34	32 (22%) 0 0	49, 66, 76, 83	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	0.51	0 100 100	25, 33, 46, 54	0
13	2R	118/118 (100%)	0.53	3 (2%) 57 61	39, 50, 60, 64	0
14	1S	110/112 (98%)	0.46	1 (0%) 84 86	37, 48, 58, 64	0
14	2S	110/112 (98%)	0.93	19 (17%) 1 1	65, 74, 79, 81	0
15	1T	131/146 (89%)	0.34	4 (3%) 49 52	33, 44, 65, 70	0
15	2T	131/146 (89%)	0.62	6 (4%) 32 34	50, 59, 71, 78	0
16	1U	116/118 (98%)	0.68	1 (0%) 84 86	21, 29, 47, 62	0
16	2U	116/118 (98%)	0.63	3 (2%) 56 59	46, 61, 74, 83	0
17	1V	101/101 (100%)	0.61	0 100 100	22, 39, 56, 64	0
17	2V	101/101 (100%)	0.43	3 (2%) 50 53	42, 70, 75, 81	0
18	1W	112/113 (99%)	0.67	0 100 100	22, 31, 50, 73	0
18	2W	112/113 (99%)	0.62	2 (1%) 68 71	40, 50, 67, 85	0
19	1X	95/96 (98%)	0.58	2 (2%) 63 66	25, 37, 56, 76	0
19	2X	95/96 (98%)	0.66	4 (4%) 36 39	45, 59, 73, 83	0
20	1Y	107/110 (97%)	0.46	0 100 100	34, 47, 64, 71	0
20	2Y	107/110 (97%)	0.81	11 (10%) 6 6	56, 69, 79, 84	0
21	1Z	154/206 (74%)	0.47	7 (4%) 33 36	38, 61, 78, 84	0
21	2Z	160/206 (77%)	0.98	29 (18%) 1 1	65, 78, 87, 89	0
22	10	83/85 (97%)	1.35	7 (8%) 11 11	27, 37, 66, 79	0
22	20	83/85 (97%)	1.33	14 (16%) 1 1	46, 65, 76, 82	0
23	11	97/98 (98%)	0.64	3 (3%) 49 52	27, 43, 66, 71	0
23	21	97/98 (98%)	0.74	5 (5%) 27 29	40, 53, 71, 75	0
24	12	70/72 (97%)	0.58	0 100 100	35, 47, 57, 70	0
24	22	70/72 (97%)	0.40	1 (1%) 75 77	59, 69, 76, 78	0
25	13	59/60 (98%)	0.52	0 100 100	24, 34, 57, 74	0
25	23	59/60 (98%)	0.88	5 (8%) 10 10	54, 64, 74, 82	0
26	14	69/71 (97%)	0.32	3 (4%) 35 38	48, 69, 83, 87	0
26	24	69/71 (97%)	1.05	15 (21%) 0 0	75, 82, 88, 95	0
27	15	59/60 (98%)	0.72	1 (1%) 70 72	20, 30, 52, 62	0
27	25	59/60 (98%)	0.43	1 (1%) 70 72	35, 49, 61, 74	0
28	16	53/54 (98%)	0.55	0 100 100	29, 42, 54, 61	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.76	6 (11%) 5 4	54, 62, 68, 73	0
29	17	48/49 (97%)	0.84	4 (8%) 11 11	21, 27, 55, 61	0
29	27	48/49 (97%)	0.97	5 (10%) 6 6	32, 42, 64, 67	0
30	18	64/65 (98%)	0.65	0 100 100	28, 34, 41, 55	0
30	28	64/65 (98%)	1.07	6 (9%) 8 8	46, 56, 62, 68	0
31	19	37/37 (100%)	0.58	0 100 100	29, 38, 54, 56	0
31	29	37/37 (100%)	1.58	11 (29%) 0 0	59, 67, 75, 76	0
32	1a	1488/1521 (97%)	0.12	39 (2%) 56 59	35, 64, 87, 99	0
32	2a	1491/1521 (98%)	0.34	90 (6%) 21 22	52, 76, 92, 101	0
33	1b	231/256 (90%)	0.33	6 (2%) 56 59	62, 74, 82, 86	0
33	2b	231/256 (90%)	1.37	60 (25%) 0 0	71, 82, 87, 89	0
34	1c	206/239 (86%)	0.47	9 (4%) 34 37	56, 68, 76, 82	0
34	2c	206/239 (86%)	1.70	79 (38%) 0 0	72, 82, 88, 93	0
35	1d	208/209 (99%)	0.84	24 (11%) 4 4	52, 68, 75, 79	0
35	2d	208/209 (99%)	1.20	40 (19%) 1 1	61, 70, 77, 80	0
36	1e	148/162 (91%)	0.52	1 (0%) 87 89	49, 62, 70, 76	0
36	2e	148/162 (91%)	1.33	39 (26%) 0 0	68, 76, 81, 87	0
37	1f	100/101 (99%)	0.42	0 100 100	52, 64, 71, 74	0
37	2f	100/101 (99%)	0.30	2 (2%) 65 68	63, 70, 75, 79	0
38	1g	155/156 (99%)	0.65	12 (7%) 13 13	56, 67, 75, 81	0
38	2g	155/156 (99%)	0.96	23 (14%) 2 2	69, 77, 83, 86	0
39	1h	137/138 (99%)	0.56	5 (3%) 42 46	53, 64, 71, 79	0
39	2h	137/138 (99%)	1.25	32 (23%) 0 0	70, 77, 81, 82	0
40	1i	127/128 (99%)	0.92	14 (11%) 5 5	49, 72, 78, 83	0
40	2i	127/128 (99%)	2.53	75 (59%) 0 0	72, 81, 86, 87	0
41	1j	97/105 (92%)	0.65	8 (8%) 11 11	58, 74, 80, 83	0
41	2j	96/105 (91%)	2.39	51 (53%) 0 0	76, 83, 87, 90	0
42	1k	114/129 (88%)	0.40	1 (0%) 84 86	45, 63, 74, 77	0
42	2k	114/129 (88%)	0.64	10 (8%) 10 10	61, 73, 79, 82	0
43	1l	121/132 (91%)	0.59	8 (6%) 18 19	45, 54, 64, 75	0
43	2l	121/132 (91%)	1.86	45 (37%) 0 0	55, 70, 77, 80	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	123/126 (97%)	0.47	9 (7%) 15 15	54, 66, 74, 84	0
44	2m	122/126 (96%)	1.80	44 (36%) 0 0	72, 80, 85, 88	0
45	1n	60/61 (98%)	1.10	7 (11%) 4 4	55, 65, 70, 74	0
45	2n	60/61 (98%)	4.23	49 (81%) 0 0	76, 83, 87, 89	0
46	1o	88/89 (98%)	0.66	9 (10%) 6 6	50, 61, 71, 74	0
46	2o	88/89 (98%)	0.77	6 (6%) 17 17	63, 72, 80, 83	0
47	1p	82/88 (93%)	1.55	27 (32%) 0 0	56, 68, 74, 82	0
47	2p	82/88 (93%)	0.99	10 (12%) 4 3	57, 67, 74, 78	0
48	1q	99/105 (94%)	0.90	11 (11%) 5 5	52, 64, 72, 76	0
48	2q	99/105 (94%)	1.28	27 (27%) 0 0	61, 71, 78, 81	0
49	1r	68/88 (77%)	0.43	3 (4%) 34 37	54, 64, 75, 77	0
49	2r	68/88 (77%)	0.44	1 (1%) 73 75	65, 72, 78, 83	0
50	1s	83/93 (89%)	0.66	4 (4%) 30 32	61, 69, 78, 81	0
50	2s	83/93 (89%)	2.50	46 (55%) 0 0	76, 84, 88, 91	0
51	1t	96/106 (90%)	1.41	30 (31%) 0 0	58, 67, 74, 79	0
51	2t	96/106 (90%)	1.42	29 (30%) 0 0	58, 69, 76, 78	0
52	1u	23/27 (85%)	1.58	7 (30%) 0 0	57, 63, 67, 71	0
52	2u	23/27 (85%)	2.73	13 (56%) 0 0	76, 79, 83, 84	0
53	1v	13/24 (54%)	1.65	4 (30%) 0 0	49, 65, 82, 92	0
53	2v	13/24 (54%)	2.62	6 (46%) 0 0	75, 83, 93, 97	0
54	1w	64/76 (84%)	2.13	22 (34%) 0 0	64, 85, 97, 101	0
54	2w	62/76 (81%)	2.94	41 (66%) 0 0	84, 92, 98, 103	0
55	1x	71/77 (92%)	0.11	0 100 100	28, 60, 80, 86	0
55	2x	71/77 (92%)	0.01	0 100 100	46, 79, 89, 90	0
56	1y	67/76 (88%)	0.57	7 (10%) 6 6	38, 85, 93, 95	0
56	2y	66/76 (86%)	1.28	16 (24%) 0 0	54, 91, 94, 98	0
All	All	20867/21748 (95%)	0.62	1700 (8%) 12 12	18, 63, 86, 103	0

All (1700) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
45	2n	34	TYR	13.8
41	2j	47	PHE	12.3

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Mol	Chain	Res	Type	RSRZ
44	2m	123	ALA	11.8
54	1w	71	G	11.6
22	10	7	LEU	10.4
54	2w	72	C	10.3
45	2n	25	VAL	10.2
45	2n	38	GLY	10.0
22	10	2	ALA	9.9
45	2n	39	LEU	9.8
22	10	3	HIS	9.7
22	10	4	LYS	9.6
50	2s	80	TYR	9.5
44	2m	124	PRO	9.1
53	2v	24	A	9.1
54	2w	73	A	9.1
50	2s	82	GLY	9.1
22	20	2	ALA	9.0
54	2w	71	G	8.9
38	2g	80	VAL	8.9
22	10	6	GLY	8.9
34	2c	157	ILE	8.9
44	1m	124	PRO	8.3
40	2i	115	GLY	8.3
38	1g	80	VAL	8.2
34	2c	194	GLY	8.2
45	2n	44	LEU	8.0
32	2a	1030(B)	C	8.0
34	2c	124	ILE	8.0
36	2e	12	LEU	8.0
54	2w	2	C	8.0
54	2w	3	C	8.0
26	24	51	ASP	7.8
40	2i	14	VAL	7.8
40	2i	7	THR	7.7
33	2b	187	LEU	7.7
38	2g	81	GLY	7.6
45	2n	42	ILE	7.6
45	2n	37	PHE	7.6
45	2n	29	ARG	7.4
43	2l	39	VAL	7.4
54	2w	31	A	7.3
26	24	49	PHE	7.2
52	2u	14	TRP	7.1

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Mol	Chain	Res	Type	RSRZ
41	2j	59	SER	7.1
34	2c	160	ALA	6.9
22	10	5	LYS	6.8
39	2h	2	LEU	6.7
45	2n	31	ARG	6.7
52	2u	6	ARG	6.7
45	2n	11	LYS	6.6
34	2c	185	GLY	6.6
50	2s	35	SER	6.6
50	2s	52	TYR	6.6
22	20	3	HIS	6.6
44	1m	123	ALA	6.5
45	2n	53	LEU	6.5
50	2s	79	THR	6.5
1	2A	2802	G	6.5
33	2b	201	ILE	6.5
41	2j	55	LYS	6.5
40	2i	114	TYR	6.4
43	2l	55	VAL	6.4
6	2G	29	TRP	6.4
22	20	7	LEU	6.4
41	2j	62	HIS	6.4
41	2j	65	LEU	6.3
44	2m	60	VAL	6.3
34	2c	198	VAL	6.3
40	2i	5	TYR	6.3
7	2H	105	LEU	6.2
53	1v	24	A	6.2
54	1w	20	U	6.2
40	2i	127	LYS	6.2
6	2G	3	LEU	6.2
44	2m	90	LEU	6.2
21	2Z	144	LEU	6.1
54	1w	70	G	6.1
54	1w	72	C	6.1
32	1a	1001(A)	G	6.1
56	2y	36	A	6.0
45	1n	2	ALA	6.0
40	2i	125	TYR	6.0
38	1g	79	ARG	6.0
52	2u	11	GLY	6.0
45	2n	8	GLU	6.0

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Mol	Chain	Res	Type	RSRZ
41	2j	63	PHE	5.9
44	2m	122	LYS	5.9
54	2w	4	C	5.8
1	1A	2159	G	5.8
43	2l	60	LEU	5.8
43	2l	32	PHE	5.8
53	2v	23	A	5.8
33	2b	70	PHE	5.7
40	2i	36	TYR	5.7
7	2H	115	VAL	5.7
33	2b	118	LEU	5.7
1	2A	2154	G	5.7
41	2j	38	ILE	5.7
54	1w	73	A	5.7
1	2A	2145	C	5.6
32	2a	1033	G	5.6
33	2b	165	VAL	5.6
7	2H	113	VAL	5.6
38	2g	154	TYR	5.6
7	2H	165	ALA	5.6
40	2i	17	VAL	5.6
45	2n	50	LYS	5.6
40	2i	76	ALA	5.6
54	2w	67	C	5.6
22	20	5	LYS	5.6
7	2H	72	ILE	5.6
40	2i	90	PRO	5.5
1	2A	2146	C	5.5
20	2Y	1	MET	5.5
32	2a	1220	G	5.5
34	2c	188	LEU	5.5
1	2A	2155	G	5.5
1	1A	1096	A	5.5
35	2d	162	LEU	5.5
1	2A	2138	C	5.5
22	20	4	LYS	5.5
7	2H	52	VAL	5.4
54	2w	70	G	5.4
7	2H	128	PRO	5.4
47	1p	1	MET	5.4
32	2a	1030(A)	G	5.4
1	2A	2147	G	5.4

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Mol	Chain	Res	Type	RSRZ
33	2b	188	ALA	5.4
56	1y	20	U	5.4
34	2c	182	ILE	5.3
34	2c	33	LEU	5.3
43	2l	56	ALA	5.3
50	2s	50	ALA	5.3
34	2c	155	GLY	5.3
34	2c	158	GLY	5.2
7	2H	35	VAL	5.2
50	2s	63	THR	5.2
44	2m	70	LEU	5.2
1	1A	1094	U	5.2
41	2j	67	THR	5.1
50	2s	41	VAL	5.1
43	2l	64	TYR	5.1
44	2m	120	LYS	5.1
7	2H	121	ILE	5.1
32	2a	1036	G	5.1
36	2e	123	LEU	5.1
40	2i	28	VAL	5.1
12	2Q	104	PHE	5.1
7	2H	102	ALA	5.1
45	2n	2	ALA	5.1
32	2a	1034	G	5.1
33	2b	92	TYR	5.1
44	2m	121	LYS	5.1
1	2A	2128	C	5.1
1	2A	2133	G	5.0
35	1d	2	GLY	5.0
39	2h	9	MET	5.0
40	2i	9	ARG	5.0
31	29	16	VAL	5.0
45	2n	6	LEU	5.0
23	2l	2	SER	5.0
56	2y	34	G	5.0
44	2m	97	PRO	5.0
7	2H	107	VAL	5.0
32	2a	1001(A)	G	5.0
50	2s	69	HIS	5.0
44	2m	102	ARG	5.0
52	2u	16	GLY	5.0
36	2e	14	ARG	5.0

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Mol	Chain	Res	Type	RSRZ
33	2b	185	ILE	5.0
40	2i	15	ALA	4.9
7	2H	94	TYR	4.9
1	2A	2127	G	4.9
29	27	48	LYS	4.9
36	2e	131	ILE	4.9
50	2s	49	ILE	4.9
41	2j	54	PHE	4.9
52	2u	15	ARG	4.9
44	2m	103	THR	4.9
1	1A	2794	C	4.8
54	1w	1	G	4.8
3	2D	2	ALA	4.8
51	1t	9	ASN	4.8
46	2o	60	VAL	4.8
44	2m	104	ARG	4.8
41	2j	72	VAL	4.8
45	2n	41	ARG	4.8
32	1a	1036	G	4.8
34	2c	159	GLY	4.8
41	2j	96	ILE	4.8
40	1i	106	ALA	4.8
44	1m	2	ALA	4.8
29	27	47	ARG	4.8
7	2H	123	PHE	4.8
41	2j	71	LEU	4.7
44	2m	23	TYR	4.7
7	2H	103	LEU	4.7
34	2c	184	TYR	4.7
40	2i	126	SER	4.7
12	2Q	65	PHE	4.7
19	2X	92	LEU	4.7
32	2a	1150	U	4.7
45	2n	7	ILE	4.7
12	2Q	121	ALA	4.6
33	2b	37	ASN	4.6
45	2n	12	ARG	4.6
38	2g	79	ARG	4.6
43	2l	68	ALA	4.6
45	2n	10	ALA	4.6
14	2S	20	ARG	4.6
45	2n	26	ARG	4.6

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Mol	Chain	Res	Type	RSRZ
35	2d	157	LEU	4.6
48	2q	80	GLY	4.6
7	2H	45	VAL	4.6
7	2H	101	ARG	4.6
34	2c	6	HIS	4.6
44	2m	87	TYR	4.6
40	2i	123	PRO	4.5
33	2b	93	VAL	4.5
12	2Q	2	LEU	4.5
44	2m	42	ALA	4.5
51	1t	12	ALA	4.5
41	2j	26	ALA	4.5
1	1A	1064	C	4.5
41	2j	40	LEU	4.5
43	1l	64	TYR	4.5
1	2A	2141	G	4.5
56	2y	57	G	4.5
21	2Z	152	ALA	4.5
8	2I	92	VAL	4.5
3	2D	276	LYS	4.5
42	2k	25	TYR	4.5
7	2H	24	VAL	4.4
35	1d	157	LEU	4.4
1	1A	885	C	4.4
1	2A	2139	C	4.4
45	2n	61	TRP	4.4
36	2e	33	VAL	4.4
33	2b	152	PHE	4.4
54	2w	14	A	4.4
54	2w	13	C	4.4
41	2j	56	HIS	4.4
7	2H	89	ILE	4.4
38	2g	40	ALA	4.4
1	2A	2174	C	4.4
45	2n	36	PHE	4.4
52	1u	17	THR	4.4
41	2j	66	ARG	4.4
44	2m	6	GLY	4.3
14	2S	12	PHE	4.3
50	2s	75	ALA	4.3
1	2A	2803	C	4.3
14	2S	14	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
36	2e	24	ARG	4.3
43	2l	95	GLY	4.3
33	2b	161	ALA	4.3
26	24	40	HIS	4.3
1	2A	2156	G	4.3
41	2j	50	ILE	4.3
32	1a	1026	G	4.3
40	2i	88	TYR	4.3
45	2n	3	ARG	4.3
54	1w	2	C	4.3
35	2d	164	ALA	4.3
45	2n	47	LEU	4.3
41	2j	48	THR	4.3
34	2c	87	LEU	4.3
26	24	63	TYR	4.2
40	2i	66	ARG	4.2
45	2n	23	ARG	4.2
50	2s	36	ARG	4.2
23	1l	98	LEU	4.2
33	2b	97	TRP	4.2
36	2e	90	VAL	4.2
38	2g	4	ARG	4.2
44	2m	66	LEU	4.2
32	1a	1028	C	4.2
1	2A	2115	G	4.2
50	2s	66	MET	4.2
8	2I	46	ALA	4.2
45	2n	14	PRO	4.2
38	2g	156	TRP	4.2
48	1q	27	PHE	4.2
7	2H	71	LEU	4.2
1	1A	2145	C	4.2
32	1a	1034	G	4.1
36	2e	130	ASN	4.1
7	2H	106	THR	4.1
45	2n	18	VAL	4.1
8	2I	75	LEU	4.1
32	2a	1224	G	4.1
32	2a	1257	U	4.1
14	2S	5	THR	4.1
43	2l	69	TYR	4.1
1	1A	2152	G	4.1

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Mol	Chain	Res	Type	RSRZ
51	1t	47	GLY	4.1
1	1A	1095	A	4.1
40	2i	102	LEU	4.1
40	2i	128	ARG	4.1
32	1a	1030(A)	G	4.1
50	2s	83	HIS	4.1
41	2j	68	HIS	4.1
1	2A	2112	G	4.1
54	1w	15	G	4.1
43	2l	41	ARG	4.1
1	1A	888	C	4.1
21	2Z	149	SER	4.1
1	2A	2801(A)	A	4.1
34	2c	200	ALA	4.1
34	2c	145	GLY	4.1
1	1A	2131	G	4.0
50	2s	70	LYS	4.0
52	2u	5	ASP	4.0
1	1A	2158	A	4.0
32	1a	1035	A	4.0
40	2i	109	VAL	4.0
45	2n	58	LYS	4.0
48	2q	6	LEU	4.0
1	2A	2793	G	4.0
44	2m	84	ILE	4.0
26	24	32	TYR	4.0
45	2n	13	THR	4.0
32	1a	1002	G	4.0
32	1a	1030(B)	C	4.0
54	1w	3	C	4.0
54	2w	5	G	4.0
1	2A	229	A	4.0
6	2G	62	LEU	4.0
40	1i	19	LEU	4.0
7	2H	37	VAL	4.0
41	2j	49	VAL	4.0
1	1A	1509	C	4.0
47	1p	59	TRP	4.0
26	24	55	ARG	4.0
44	2m	94	ARG	4.0
45	2n	40	CYS	4.0
50	2s	40	ILE	4.0

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Mol	Chain	Res	Type	RSRZ
1	2A	652(B)	A	4.0
35	2d	160	GLN	4.0
7	2H	7	LEU	3.9
32	1a	1027	C	3.9
21	2Z	156	LYS	3.9
21	2Z	170	THR	3.9
6	2G	136	ARG	3.9
34	2c	12	LEU	3.9
41	2j	88	LEU	3.9
51	2t	63	ILE	3.9
31	29	37	GLY	3.9
50	2s	53	ASN	3.9
8	2l	35	LEU	3.9
50	2s	71	LEU	3.9
40	2i	63	ILE	3.9
41	2j	98	ILE	3.9
34	2c	65	ALA	3.9
50	2s	13	ASP	3.9
51	2t	73	HIS	3.9
12	2Q	22	LYS	3.9
35	1d	138	TYR	3.9
32	1a	1003	G	3.9
33	2b	48	MET	3.9
1	2A	2111	C	3.9
1	2A	2804	C	3.9
32	2a	1030	C	3.9
39	2h	93	VAL	3.9
50	1s	71	LEU	3.9
51	1t	13	LEU	3.9
44	2m	101	GLN	3.9
38	1g	82	GLY	3.8
45	2n	15	LYS	3.8
1	2A	2109	U	3.8
21	2Z	153	SER	3.8
40	2i	26	VAL	3.8
21	2Z	155	LEU	3.8
39	2h	94	TYR	3.8
51	1t	74	LYS	3.8
1	2A	1026	U	3.8
40	2i	83	ARG	3.8
53	2v	22	U	3.8
1	1A	2151	G	3.8

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Mol	Chain	Res	Type	RSRZ
7	2H	157	TYR	3.8
36	2e	13	ILE	3.8
1	1A	2132	U	3.8
54	1w	14	A	3.8
12	2Q	37	LEU	3.8
48	2q	22	LEU	3.8
51	2t	24	LEU	3.8
33	2b	71	VAL	3.8
51	1t	72	LEU	3.8
1	2A	2160	G	3.8
6	1G	146	TYR	3.8
23	1l	2	SER	3.8
44	2m	78	ILE	3.8
50	2s	38	SER	3.8
38	1g	85	TYR	3.8
32	1a	1030(C)	G	3.8
32	2a	1002	G	3.8
54	1w	44	G	3.8
54	2w	65	G	3.8
44	2m	88	ARG	3.7
45	2n	4	LYS	3.7
32	2a	1061	G	3.7
40	2i	105	ASP	3.7
32	1a	1531	A	3.7
54	2w	38	A	3.7
36	2e	109	ILE	3.7
39	2h	86	ILE	3.7
39	2h	4	ASP	3.7
39	2h	112	LEU	3.7
39	2h	131	GLY	3.7
6	2G	140	ILE	3.7
34	2c	8	ILE	3.7
32	1a	1532	U	3.7
33	2b	81	VAL	3.7
36	2e	10	MET	3.7
56	1y	35	A	3.7
33	2b	51	LEU	3.7
53	2v	21	C	3.7
50	2s	37	ARG	3.7
1	1A	2160	G	3.7
54	1w	31	A	3.7
40	2i	82	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
50	2s	14	HIS	3.7
33	2b	163	PHE	3.7
7	2H	6	ARG	3.7
34	2c	91	LEU	3.7
46	1o	57	LEU	3.7
45	2n	22	THR	3.7
29	27	1	MET	3.7
32	1a	163	C	3.7
54	1w	13	C	3.7
43	2l	31	PRO	3.6
21	2Z	5	LEU	3.6
33	2b	177	ALA	3.6
33	2b	101	MET	3.6
40	2i	81	ILE	3.6
32	2a	1219	U	3.6
40	2i	57	GLY	3.6
41	2j	51	ARG	3.6
45	2n	35	ARG	3.6
32	2a	1018	C	3.6
35	2d	180	GLY	3.6
47	1p	19	ILE	3.6
3	2D	38	LYS	3.6
32	1a	204	U	3.6
6	2G	152	LEU	3.6
7	2H	124	GLU	3.6
14	2S	32	LEU	3.6
50	2s	84	GLY	3.6
48	1q	36	ILE	3.6
19	2X	68	ARG	3.6
51	1t	22	ARG	3.6
40	2i	20	ARG	3.6
45	2n	27	CYS	3.6
48	1q	98	LEU	3.6
51	2t	20	LEU	3.6
54	2w	56	C	3.6
11	2P	149	GLU	3.6
40	2i	122	ALA	3.6
21	2Z	139	VAL	3.6
14	2S	29	PHE	3.5
44	2m	4	ILE	3.5
48	2q	36	ILE	3.5
34	2c	52	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
38	2g	84	ASN	3.5
40	2i	27	THR	3.5
41	2j	93	GLY	3.5
54	1w	69	G	3.5
7	2H	36	PRO	3.5
34	2c	39	ILE	3.5
36	2e	84	PHE	3.5
1	1A	1066	U	3.5
32	2a	1363(A)	A	3.5
33	2b	69	LEU	3.5
33	2b	227	GLY	3.5
43	2l	77	LEU	3.5
1	1A	2141	G	3.5
32	2a	1030(C)	G	3.5
47	2p	19	ILE	3.5
35	2d	168	ARG	3.5
51	2t	76	ALA	3.5
43	2l	101	VAL	3.5
14	2S	92	TYR	3.5
38	2g	85	TYR	3.5
47	1p	80	PHE	3.5
1	1A	2109	U	3.5
45	2n	55	GLY	3.5
47	1p	37	GLY	3.5
50	2s	68	GLY	3.5
6	1G	139	LEU	3.5
7	2H	98	LEU	3.5
7	2H	44	VAL	3.5
12	2Q	113	GLN	3.5
40	2i	59	PHE	3.5
6	2G	19	LEU	3.5
21	2Z	125	LEU	3.5
50	2s	77	THR	3.5
54	2w	15	G	3.5
6	2G	73	ALA	3.5
40	2i	67	GLY	3.5
34	2c	202	ILE	3.5
51	2t	72	LEU	3.5
7	2H	159	GLU	3.5
43	2l	82	VAL	3.5
51	2t	9	ASN	3.5
34	2c	193	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
43	2l	120	TYR	3.4
47	1p	39	TYR	3.4
33	2b	162	ILE	3.4
35	2d	158	ILE	3.4
51	1t	55	ILE	3.4
12	2Q	5	ARG	3.4
43	2l	93	LEU	3.4
34	2c	4	LYS	3.4
44	2m	119	GLY	3.4
32	2a	1357	A	3.4
38	2g	42	ILE	3.4
40	2i	101	PHE	3.4
51	2t	22	ARG	3.4
7	2H	82	GLY	3.4
1	2A	2143	C	3.4
41	2j	61	GLU	3.4
40	2i	121	ARG	3.4
6	2G	182	LYS	3.4
34	2c	167	TRP	3.4
7	2H	57	ASP	3.4
22	10	8	GLY	3.4
34	2c	28	GLN	3.4
7	2H	19	VAL	3.4
45	2n	56	VAL	3.4
35	2d	146	ILE	3.4
1	1A	2897	U	3.4
1	2A	2132	U	3.4
32	2a	1358	U	3.4
47	1p	7	ALA	3.4
7	2H	55	PRO	3.4
32	1a	1030(D)	A	3.4
53	1v	12	A	3.4
8	2I	82	ARG	3.4
36	2e	99	GLY	3.4
48	2q	91	ARG	3.4
54	2w	50	U	3.4
32	2a	1356	G	3.4
41	2j	74	ILE	3.3
40	2i	75	ASP	3.3
45	2n	24	CYS	3.3
35	1d	3	ARG	3.3
35	1d	122	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
6	2G	28	VAL	3.3
26	24	50	VAL	3.3
32	2a	1026	G	3.3
47	2p	74	LEU	3.3
3	1D	2	ALA	3.3
41	2j	12	ASP	3.3
10	2O	1	MET	3.3
36	2e	8	GLU	3.3
34	2c	207	VAL	3.3
41	1j	44	VAL	3.3
29	27	23	ARG	3.3
50	2s	81	ARG	3.3
51	2t	25	ARG	3.3
34	2c	170	GLN	3.3
31	29	25	VAL	3.3
45	2n	57	ARG	3.3
39	2h	83	ILE	3.3
32	2a	973	G	3.3
27	15	60	VAL	3.3
51	2t	83	ARG	3.3
40	2i	19	LEU	3.3
32	1a	1001	A	3.3
41	2j	32	ALA	3.3
22	20	6	GLY	3.3
1	2A	883	G	3.3
6	2G	48	GLU	3.3
35	2d	115	ARG	3.3
7	2H	96	ALA	3.3
12	2Q	66	ILE	3.3
34	2c	189	ALA	3.3
44	2m	92	HIS	3.3
1	2A	888	C	3.3
32	2a	1027	C	3.3
36	2e	22	GLY	3.3
22	20	77	ARG	3.3
3	1D	276	LYS	3.3
30	28	29	LYS	3.3
43	2l	13	LYS	3.3
21	1Z	141	VAL	3.3
44	2m	98	VAL	3.3
1	2A	2110	G	3.2
32	1a	1024	G	3.2

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Mol	Chain	Res	Type	RSRZ
7	2H	92	ILE	3.2
45	2n	46	GLU	3.2
47	1p	30	GLY	3.2
33	2b	193	ASP	3.2
1	1A	896	A	3.2
1	2A	2129	C	3.2
32	2a	994	A	3.2
32	2a	1035	A	3.2
32	2a	1218	C	3.2
47	1p	66	PRO	3.2
1	1A	1093	G	3.2
1	2A	2152	G	3.2
22	20	69	PHE	3.2
40	2i	46	ALA	3.2
32	1a	1257	U	3.2
32	2a	1040	U	3.2
35	1d	70	ILE	3.2
44	2m	9	ILE	3.2
44	1m	122	LYS	3.2
34	2c	37	GLN	3.2
56	1y	36	A	3.2
7	2H	125	VAL	3.2
7	2H	133	VAL	3.2
12	2Q	6	ARG	3.2
45	2n	59	ALA	3.2
26	14	59	PHE	3.2
1	2A	2118	U	3.2
36	2e	29	GLY	3.2
41	2j	44	VAL	3.2
44	1m	98	VAL	3.2
7	2H	145	ALA	3.2
36	2e	104	ALA	3.2
1	2A	2144	U	3.2
41	2j	6	ILE	3.2
8	2I	1	MET	3.2
32	1a	1033	G	3.2
7	2H	74	ASN	3.2
7	2H	166	GLY	3.2
34	2c	64	VAL	3.2
47	1p	24	ALA	3.2
7	2H	4	ILE	3.2
33	2b	214	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
39	2h	35	ILE	3.2
38	2g	32	ARG	3.2
47	1p	27	LYS	3.2
51	2t	29	LYS	3.2
21	2Z	145	GLU	3.2
40	2i	110	GLU	3.2
43	2l	88	GLY	3.2
7	2H	49	VAL	3.2
1	1A	2803	C	3.2
6	2G	146	TYR	3.2
50	2s	48	THR	3.2
51	1t	24	LEU	3.2
51	1t	80	ARG	3.2
14	2S	31	SER	3.2
21	1Z	149	SER	3.2
8	2I	19	VAL	3.2
6	2G	110	ALA	3.1
11	2P	45	LEU	3.2
34	1c	193	TYR	3.1
34	2c	191	THR	3.1
35	2d	135	LEU	3.2
54	2w	40	C	3.1
21	2Z	124	ILE	3.1
32	2a	1532	U	3.1
34	2c	5	ILE	3.1
41	2j	58	ASP	3.1
54	2w	66	U	3.1
21	2Z	50	GLN	3.1
35	2d	6	GLY	3.1
43	2l	19	ARG	3.1
7	2H	99	VAL	3.1
7	2H	114	VAL	3.1
8	2I	38	LEU	3.1
48	2q	11	VAL	3.1
51	1t	67	ALA	3.1
1	2A	2175	C	3.1
40	2i	117	HIS	3.1
56	2y	15	G	3.1
32	1a	162	A	3.1
12	2Q	97	VAL	3.1
43	1l	18	VAL	3.1
47	1p	2	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
7	2H	108	GLY	3.1
6	2G	178	PHE	3.1
12	2Q	69	PHE	3.1
1	1A	2140	C	3.1
32	2a	1149	C	3.1
54	2w	19	G	3.1
12	2Q	106	VAL	3.1
33	2b	67	THR	3.1
41	2j	64	GLU	3.1
1	1A	2130	U	3.1
10	2O	69	ILE	3.1
32	1a	1025	U	3.1
29	17	48	LYS	3.1
32	1a	1029	C	3.1
43	2l	28	LYS	3.1
1	1A	2112	G	3.1
32	2a	1021	G	3.1
14	2S	54	LEU	3.1
36	2e	43	LEU	3.1
39	2h	10	LEU	3.1
36	2e	55	VAL	3.1
40	2i	103	THR	3.1
47	1p	6	LEU	3.1
51	2t	8	ARG	3.1
8	2I	37	VAL	3.1
34	2c	14	ILE	3.1
40	2i	124	GLN	3.1
35	1d	73	ARG	3.1
40	2i	64	THR	3.1
34	2c	153	VAL	3.1
40	2i	65	VAL	3.1
1	2A	2125	G	3.1
32	1a	1031	G	3.1
32	2a	1202	G	3.1
54	1w	10	G	3.1
1	2A	2113	U	3.1
44	2m	10	PRO	3.1
40	2i	93	ARG	3.1
41	2j	60	ARG	3.1
40	1i	113	LYS	3.1
40	2i	80	GLY	3.1
17	2V	72	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
40	2i	108	VAL	3.1
44	2m	7	VAL	3.1
33	2b	232	PRO	3.0
1	1A	1068	G	3.0
34	2c	186	PHE	3.0
35	2d	73	ARG	3.0
41	2j	45	ARG	3.0
43	2l	100	ILE	3.0
41	2j	52	GLY	3.0
40	1i	15	ALA	3.0
45	2n	49	HIS	3.0
40	1i	65	VAL	3.0
39	2h	92	ARG	3.0
40	2i	49	PRO	3.0
40	2i	18	PHE	3.0
39	2h	58	TYR	3.0
11	2P	79	ARG	3.0
35	2d	159	ARG	3.0
43	2l	51	ALA	3.0
1	1A	2129	C	3.0
1	1A	271(K)	U	3.0
41	2j	11	PHE	3.0
45	2n	16	PHE	3.0
46	1o	36	ILE	3.0
38	2g	82	GLY	3.0
14	2S	3	ARG	3.0
38	1g	42	ILE	3.0
38	1g	81	GLY	3.0
40	2i	77	ILE	3.0
52	2u	2	GLY	3.0
40	2i	40	LEU	3.0
43	2l	27	LEU	3.0
44	2m	48	LEU	3.0
51	1t	76	ALA	3.0
1	2A	2116	G	3.0
1	2A	2153	G	3.0
54	2w	69	G	3.0
33	1b	133	LYS	3.0
34	2c	13	GLY	3.0
44	2m	100	GLY	3.0
7	2H	51	ARG	3.0
56	1y	56	C	3.0

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Mol	Chain	Res	Type	RSRZ
36	2e	45	PHE	3.0
10	2O	81	ASP	3.0
38	2g	16	LEU	3.0
51	2t	66	ALA	3.0
7	2H	95	ARG	3.0
43	1l	29	GLY	3.0
51	2t	26	ASN	3.0
16	2U	17	ILE	3.0
50	2s	62	ILE	3.0
40	2i	79	LEU	3.0
50	2s	15	LEU	3.0
33	1b	227	GLY	3.0
40	2i	8	GLY	3.0
44	2m	110	ARG	3.0
39	2h	61	VAL	2.9
12	2Q	103	MET	2.9
54	2w	47	U	2.9
7	2H	83	TYR	2.9
34	2c	192	THR	2.9
40	2i	62	TYR	2.9
34	2c	41	GLY	2.9
20	2Y	91	GLU	2.9
7	2H	30	LYS	2.9
20	2Y	5	MET	2.9
9	2N	60	ILE	2.9
56	2y	33	U	2.9
51	1t	18	GLN	2.9
32	2a	1115	C	2.9
11	2P	6	LEU	2.9
20	2Y	65	ALA	2.9
32	1a	1032	G	2.9
39	2h	28	ALA	2.9
33	2b	31	TYR	2.9
39	2h	36	LEU	2.9
46	2o	66	LEU	2.9
47	1p	60	LEU	2.9
48	1q	28	PRO	2.9
51	1t	73	HIS	2.9
53	1v	23	A	2.9
4	2E	134	ILE	2.9
6	2G	102	PHE	2.9
35	2d	70	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
9	2N	112	LEU	2.9
23	2I	68	PRO	2.9
32	2a	1114	C	2.9
44	2m	96	LEU	2.9
52	2u	21	TYR	2.9
35	2d	112	VAL	2.9
50	2s	67	VAL	2.9
51	2t	17	ARG	2.9
32	2a	969	A	2.9
39	2h	134	ILE	2.9
47	2p	48	TRP	2.9
33	2b	72	GLY	2.9
35	2d	167	GLY	2.9
51	1t	68	LYS	2.9
32	1a	1030	C	2.9
26	24	35	VAL	2.9
36	2e	34	VAL	2.9
44	2m	15	VAL	2.9
47	1p	20	VAL	2.9
3	2D	275	LYS	2.9
32	2a	1003	G	2.9
47	1p	33	ILE	2.9
52	2u	23	PRO	2.9
6	2G	161	THR	2.9
7	2H	129	THR	2.9
8	2I	12	LEU	2.9
33	2b	90	MET	2.9
47	1p	21	VAL	2.9
50	2s	4	SER	2.9
12	2Q	19	GLY	2.9
1	1A	1060	U	2.9
1	2A	2159	G	2.9
4	2E	77	ILE	2.9
32	2a	1221	G	2.9
54	2w	44	G	2.9
40	2i	42	ARG	2.9
51	1t	89	ARG	2.9
54	2w	7	A	2.9
7	2H	172	LYS	2.9
20	2Y	90	LEU	2.9
33	2b	121	LEU	2.9
51	2t	71	THR	2.9

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Mol	Chain	Res	Type	RSRZ
48	2q	95	TYR	2.9
1	1A	2128	C	2.8
1	1A	2174	C	2.8
9	2N	9	VAL	2.8
21	2Z	143	GLY	2.8
40	2i	53	VAL	2.8
51	1t	75	ASN	2.8
34	2c	21	ARG	2.8
1	1A	1081	U	2.8
1	2A	271(K)	U	2.8
3	2D	5	LYS	2.8
38	2g	27	ILE	2.8
1	1A	1057	A	2.8
1	1A	1087	G	2.8
1	2A	2173	A	2.8
7	2H	64	LEU	2.8
39	2h	26	VAL	2.8
6	2G	41	GLN	2.8
34	2c	134	ILE	2.8
39	2h	45	ILE	2.8
43	2l	30	ALA	2.8
35	1d	21	LEU	2.8
1	2A	2126	A	2.8
32	2a	983	A	2.8
32	2a	1031	G	2.8
35	1d	159	ARG	2.8
41	2j	10	GLY	2.8
54	1w	30	G	2.8
6	2G	159	VAL	2.8
21	2Z	96	VAL	2.8
21	2Z	141	VAL	2.8
36	2e	20	GLN	2.8
40	2i	86	VAL	2.8
50	2s	60	VAL	2.8
8	2I	88	ILE	2.8
54	1w	68	C	2.8
8	2I	47	LEU	2.8
33	2b	44	LEU	2.8
51	1t	62	LEU	2.8
35	1d	209	ARG	2.8
36	2e	107	ARG	2.8
40	2i	10	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
41	1j	46	ARG	2.8
44	2m	91	ARG	2.8
7	2H	2	SER	2.8
9	2N	69	GLN	2.8
32	2a	1225	A	2.8
32	2a	1286	A	2.8
56	2y	21	A	2.8
6	2G	11	TYR	2.8
1	1A	2108	C	2.8
7	2H	3	ARG	2.8
32	2a	1116	C	2.8
32	2a	1223	C	2.8
54	1w	25	C	2.8
11	2P	59	LEU	2.8
35	2d	120	LEU	2.8
9	2N	8	GLN	2.8
18	2W	112	GLY	2.8
7	2H	76	VAL	2.8
32	2a	1001	A	2.8
43	1l	91	LYS	2.8
7	2H	9	ILE	2.8
11	2P	91	PHE	2.8
36	2e	76	ILE	2.8
40	2i	43	ALA	2.8
1	2A	885	C	2.8
7	2H	88	LEU	2.8
25	23	23	LEU	2.8
32	1a	1037	C	2.8
35	2d	23	GLY	2.8
34	2c	206	GLU	2.8
39	2h	133	LEU	2.8
41	1j	10	GLY	2.8
51	2t	36	LEU	2.8
35	2d	122	ARG	2.8
7	2H	169	VAL	2.8
31	29	12	ASP	2.8
48	2q	73	VAL	2.8
32	1a	161	A	2.8
14	2S	40	ILE	2.8
34	1c	124	ILE	2.8
39	2h	3	THR	2.8
48	2q	44	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	2A	2124	G	2.8
19	1X	95	LEU	2.8
54	2w	24	G	2.8
35	2d	18	LYS	2.8
1	1A	2138	C	2.8
40	1i	126	SER	2.8
41	2j	46	ARG	2.8
25	23	60	GLU	2.7
1	2A	896	A	2.7
12	2Q	68	ILE	2.7
32	2a	1044	A	2.7
40	2i	74	ILE	2.7
4	2E	195	LEU	2.7
35	1d	115	ARG	2.7
51	1t	83	ARG	2.7
1	1A	1076	C	2.7
1	1A	2111	C	2.7
32	2a	1038	C	2.7
21	2Z	167	PRO	2.7
51	1t	16	HIS	2.7
34	2c	72	LYS	2.7
34	2c	2	GLY	2.7
1	2A	2167	U	2.7
22	20	45	PHE	2.7
47	1p	17	TYR	2.7
36	2e	31	LEU	2.7
7	2H	111	HIS	2.7
1	1A	2115	G	2.7
1	1A	2161	C	2.7
1	2A	2136	C	2.7
1	2A	2805	G	2.7
54	2w	10	G	2.7
54	2w	41	C	2.7
6	1G	48	GLU	2.7
7	2H	148	ILE	2.7
20	2Y	89	PHE	2.7
30	28	41	ILE	2.7
35	2d	20	TYR	2.7
39	2h	65	TYR	2.7
40	2i	33	PHE	2.7
50	2s	31	ILE	2.7
9	2N	23	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
13	2R	65	LEU	2.7
50	1s	15	LEU	2.7
45	2n	54	PRO	2.7
26	24	54	GLY	2.7
32	2a	980	C	2.7
34	2c	190	ARG	2.7
12	2Q	109	VAL	2.7
38	1g	83	ALA	2.7
7	2H	56	SER	2.7
14	2S	35	ILE	2.7
14	2S	52	SER	2.7
36	2e	125	SER	2.7
39	2h	111	ILE	2.7
6	1G	21	ARG	2.7
7	2H	132	ARG	2.7
35	1d	23	GLY	2.7
39	2h	135	CYS	2.7
32	2a	1397	C	2.7
45	2n	33	VAL	2.7
10	2O	65	THR	2.7
44	2m	105	THR	2.7
1	2A	2123	G	2.7
11	2P	75	ILE	2.7
30	28	61	LEU	2.7
40	2i	37	PHE	2.7
51	2t	41	ILE	2.7
54	2w	6	G	2.7
12	2Q	32	TYR	2.7
21	2Z	151	HIS	2.7
51	1t	69	GLY	2.7
52	1u	11	GLY	2.7
32	2a	1092	A	2.7
1	2A	2161	C	2.7
34	2c	19	GLU	2.7
12	2Q	29	PHE	2.7
31	29	32	HIS	2.7
40	1i	81	ILE	2.7
46	2o	31	LEU	2.7
49	1r	78	LEU	2.7
52	2u	24	ARG	2.7
1	2A	2162	G	2.7
32	1a	1023	G	2.7

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Mol	Chain	Res	Type	RSRZ
32	2a	998	G	2.7
33	2b	14	GLY	2.7
7	2H	10	PRO	2.7
30	28	34	TRP	2.7
26	24	57	GLU	2.6
36	2e	81	GLU	2.6
8	2I	3	VAL	2.6
33	2b	197	VAL	2.6
36	2e	16	THR	2.6
33	2b	155	LEU	2.6
35	1d	135	LEU	2.6
39	1h	127	LEU	2.6
43	1l	7	ILE	2.6
47	2p	4	ILE	2.6
8	2I	34	GLY	2.6
38	1g	154	TYR	2.6
6	2G	35	GLU	2.6
1	2A	2894	G	2.6
32	2a	1024	G	2.6
40	1i	14	VAL	2.6
26	24	27	THR	2.6
16	2U	43	GLY	2.6
25	23	53	LEU	2.6
34	1c	39	ILE	2.6
35	1d	5	ILE	2.6
35	2d	16	GLY	2.6
43	2l	25	PRO	2.6
19	2X	69	TYR	2.6
33	2b	139	LYS	2.6
29	17	46	VAL	2.6
32	2a	1190	G	2.6
33	2b	210	SER	2.6
36	2e	105	VAL	2.6
38	2g	147	ALA	2.6
39	2h	95	VAL	2.6
54	2w	52	G	2.6
56	1y	19	G	2.6
7	2H	48	GLY	2.6
36	2e	114	GLY	2.6
1	2A	2170	A	2.6
12	2Q	79	LEU	2.6
47	1p	65	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
48	2q	98	LEU	2.6
32	2a	1039	C	2.6
56	2y	56	C	2.6
41	2j	36	GLY	2.6
48	2q	21	VAL	2.6
11	2P	76	LYS	2.6
1	1A	1065	U	2.6
1	2A	614(B)	G	2.6
38	2g	22	LEU	2.6
40	2i	116	LYS	2.6
54	1w	47	U	2.6
46	2o	87	ILE	2.6
48	2q	59	ILE	2.6
32	2a	1250	A	2.6
54	2w	68	C	2.6
21	1Z	166	SER	2.6
35	2d	52	SER	2.6
7	2H	100	GLY	2.6
46	1o	89	GLY	2.6
33	2b	220	ASP	2.6
43	2l	59	ARG	2.6
50	2s	11	VAL	2.6
52	2u	8	THR	2.6
1	1A	1082	U	2.6
31	29	26	ILE	2.6
52	1u	14	TRP	2.6
32	2a	1032	G	2.6
54	2w	30	G	2.6
32	2a	977	A	2.6
7	2H	138	LYS	2.6
11	2P	109	GLY	2.6
35	2d	183	GLY	2.6
29	17	47	ARG	2.6
35	2d	49	ARG	2.6
40	2i	16	ARG	2.6
8	2I	93	THR	2.6
48	2q	7	THR	2.6
51	2t	77	ALA	2.6
15	2T	102	ILE	2.6
34	2c	152	ILE	2.6
50	2s	56	GLN	2.6
1	1A	1059	G	2.6

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Mol	Chain	Res	Type	RSRZ
22	20	44	ARG	2.6
46	2o	61	GLY	2.6
7	2H	122	THR	2.5
34	2c	53	ALA	2.5
36	2e	17	ALA	2.5
20	2Y	24	VAL	2.5
48	2q	9	VAL	2.5
50	2s	33	THR	2.5
50	2s	45	VAL	2.5
35	2d	94	LEU	2.5
44	1m	90	LEU	2.5
32	2a	961	U	2.5
8	2l	97	ILE	2.5
15	2T	75	ILE	2.5
33	2b	122	PHE	2.5
41	1j	5	ARG	2.5
51	1t	79	ARG	2.5
38	1g	156	TRP	2.5
1	1A	1099	G	2.5
35	1d	207	TYR	2.5
35	2d	106	TYR	2.5
42	2k	59	TYR	2.5
44	2m	5	ALA	2.5
1	2A	2896	C	2.5
32	2a	1028	C	2.5
7	2H	67	LEU	2.5
35	1d	120	LEU	2.5
51	1t	20	LEU	2.5
28	26	7	ILE	2.5
35	1d	110	PHE	2.5
31	29	13	LYS	2.5
3	2D	153	ALA	2.5
7	2H	112	PRO	2.5
43	2l	71	PRO	2.5
6	2G	34	LEU	2.5
15	2T	78	LEU	2.5
56	2y	18	G	2.5
11	2P	51	PHE	2.5
33	2b	57	PHE	2.5
34	2c	69	HIS	2.5
43	2l	72	GLY	2.5
47	1p	4	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
47	2p	80	PHE	2.5
51	2t	55	ILE	2.5
34	1c	180	ALA	2.5
34	2c	149	ALA	2.5
50	2s	78	ARG	2.5
52	2u	10	ARG	2.5
6	2G	133	LEU	2.5
6	2G	149	VAL	2.5
28	26	34	LEU	2.5
32	1a	1503	A	2.5
34	2c	199	LYS	2.5
1	1A	1100	C	2.5
1	2A	2897	U	2.5
35	2d	69	GLY	2.5
1	2A	1816	G	2.5
6	2G	39	ILE	2.5
39	2h	124	ALA	2.5
21	2Z	154	ASP	2.5
45	1n	61	TRP	2.5
50	2s	34	TRP	2.5
3	2D	18	VAL	2.5
15	1T	114	LEU	2.5
33	1b	228	GLY	2.5
43	2l	84	LEU	2.5
46	1o	69	TYR	2.5
52	1u	21	TYR	2.5
1	1A	1098	A	2.5
1	2A	6	A	2.5
1	2A	2117	A	2.5
32	2a	1287	A	2.5
53	2v	12	A	2.5
12	2Q	64	ILE	2.5
20	2Y	44	ILE	2.5
34	2c	143	GLU	2.5
45	2n	19	ARG	2.5
45	2n	45	ARG	2.5
8	2I	21	VAL	2.5
10	2O	38	VAL	2.5
34	2c	48	TYR	2.5
44	1m	87	TYR	2.5
7	2H	84	SER	2.5
14	2S	13	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
25	23	29	ARG	2.5
1	1A	2117	A	2.5
19	2X	28	PHE	2.5
43	2l	46	LYS	2.5
22	20	76	GLY	2.5
14	2S	58	LEU	2.4
15	2T	111	ARG	2.4
52	2u	22	ARG	2.4
7	2H	144	VAL	2.4
7	2H	163	TYR	2.4
26	24	43	TYR	2.4
51	1t	70	SER	2.4
22	20	57	PHE	2.4
30	28	48	PHE	2.4
12	2Q	33	GLY	2.4
47	1p	41	PRO	2.4
14	2S	34	HIS	2.4
38	2g	6	ARG	2.4
1	1A	1058	G	2.4
7	2H	171	LEU	2.4
43	2l	10	LEU	2.4
48	2q	23	VAL	2.4
1	1A	1078	U	2.4
26	14	57	GLU	2.4
6	2G	86	MET	2.4
38	2g	26	PHE	2.4
42	2k	125	PHE	2.4
8	2I	13	GLY	2.4
33	2b	94	ASN	2.4
1	1A	1077	A	2.4
12	1Q	6	ARG	2.4
12	1Q	59	ARG	2.4
36	2e	9	LYS	2.4
48	2q	92	ARG	2.4
1	2A	2137	C	2.4
1	2A	2140	C	2.4
54	2w	49	C	2.4
12	2Q	17	LEU	2.4
43	2l	110	VAL	2.4
45	1n	33	VAL	2.4
32	2a	951	G	2.4
9	2N	85	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
48	2q	90	ILE	2.4
34	2c	59	ARG	2.4
9	2N	22	THR	2.4
28	26	2	ALA	2.4
34	2c	20	SER	2.4
22	20	79	VAL	2.4
25	23	54	VAL	2.4
35	1d	105	VAL	2.4
41	2j	34	VAL	2.4
41	2j	94	VAL	2.4
50	2s	51	VAL	2.4
44	2m	99	ARG	2.4
6	2G	77	ILE	2.4
8	2I	4	ILE	2.4
41	1j	98	ILE	2.4
44	2m	25	ILE	2.4
48	2q	42	TYR	2.4
41	2j	87	THR	2.4
47	1p	67	THR	2.4
12	2Q	10	ARG	2.4
32	2a	1016	A	2.4
41	2j	85	LEU	2.4
48	1q	31	LEU	2.4
33	2b	53	ARG	2.4
33	1b	71	VAL	2.4
8	2I	79	ILE	2.4
12	2Q	47	ILE	2.4
48	2q	65	ILE	2.4
42	2k	121	PRO	2.4
44	1m	121	LYS	2.4
2	2B	119	G	2.4
41	2j	15	THR	2.4
35	1d	118	ARG	2.4
38	2g	3	ARG	2.4
42	2k	126	ARG	2.4
51	1t	8	ARG	2.4
7	2H	33	LEU	2.4
46	1o	56	LEU	2.4
32	2a	965	A	2.4
42	2k	117	ASN	2.4
52	1u	16	GLY	2.4
7	2H	41	MET	2.4

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Mol	Chain	Res	Type	RSRZ
31	29	17	ILE	2.4
35	1d	206	PHE	2.4
43	2l	94	PRO	2.4
43	2l	99	HIS	2.4
52	1u	13	ILE	2.4
21	2Z	8	TYR	2.4
6	2G	95	ARG	2.4
40	2i	61	ALA	2.4
34	2c	177	THR	2.4
11	1P	100	LEU	2.4
12	2Q	34	LEU	2.4
1	2A	2131	G	2.3
32	2a	953	G	2.3
34	2c	181	ASN	2.3
34	2c	150	LYS	2.3
20	2Y	45	VAL	2.3
37	2f	40	VAL	2.3
1	1A	884	C	2.3
36	2e	89	ILE	2.3
41	1j	41	PRO	2.3
7	2H	97	ARG	2.3
41	2j	70	ARG	2.3
52	1u	6	ARG	2.3
35	2d	207	TYR	2.3
7	2H	53	GLU	2.3
44	2m	69	GLU	2.3
8	2I	74	ASN	2.3
12	1Q	79	LEU	2.3
33	2b	215	LEU	2.3
34	1c	34	LEU	2.3
34	2c	171	GLY	2.3
43	1l	63	GLY	2.3
51	2t	13	LEU	2.3
7	2H	65	HIS	2.3
39	2h	19	VAL	2.3
12	2Q	59	ARG	2.3
43	2l	65	GLU	2.3
14	2S	37	ALA	2.3
11	2P	32	THR	2.3
48	1q	7	THR	2.3
35	2d	78	LEU	2.3
40	2i	107	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
48	1q	38	ARG	2.3
7	2H	46	GLU	2.3
21	2Z	126	VAL	2.3
36	2e	67	VAL	2.3
43	2l	5	PRO	2.3
43	2l	43	VAL	2.3
39	2h	32	LYS	2.3
44	2m	82	MET	2.3
1	1A	2146	C	2.3
1	1A	2190	G	2.3
32	2a	1006	C	2.3
6	2G	61	ALA	2.3
7	2H	16	SER	2.3
21	1Z	51	ALA	2.3
21	2Z	21	ALA	2.3
34	2c	100	ALA	2.3
34	2c	187	ALA	2.3
7	2H	58	GLU	2.3
9	2N	61	ARG	2.3
10	2O	106	LEU	2.3
46	1o	39	LEU	2.3
50	2s	57	HIS	2.3
43	2l	24	VAL	2.3
43	2l	96	VAL	2.3
47	2p	59	TRP	2.3
29	17	1	MET	2.3
7	2H	151	ILE	2.3
7	2H	47	GLU	2.3
12	2Q	40	ALA	2.3
21	2Z	99	TYR	2.3
32	2a	91	C	2.3
32	2a	976	G	2.3
32	2a	1321	C	2.3
33	2b	62	ALA	2.3
33	2b	203	GLY	2.3
54	2w	11	C	2.3
32	2a	1251	A	2.3
54	2w	22	G	2.3
56	2y	35	A	2.3
8	2I	140	LEU	2.3
40	1i	56	LEU	2.3
50	2s	30	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
43	2l	18	VAL	2.3
7	2H	78	GLY	2.3
8	1I	79	ILE	2.3
33	1b	68	ILE	2.3
34	2c	30	ARG	2.3
36	1e	89	ILE	2.3
43	2l	29	GLY	2.3
51	1t	86	ARG	2.3
36	2e	21	ALA	2.3
45	1n	48	ALA	2.3
51	2t	12	ALA	2.3
51	2t	32	ALA	2.3
34	2c	17	ASP	2.3
21	1Z	102	LEU	2.3
32	2a	1048	G	2.3
32	2a	1229	A	2.3
34	2c	47	LEU	2.3
1	2A	2166	G	2.3
2	2B	118	G	2.3
53	1v	13	A	2.3
54	2w	28	G	2.3
56	2y	23	A	2.3
21	2Z	68	PRO	2.3
33	2b	202	PRO	2.3
1	1A	1026	U	2.3
12	2Q	60	ARG	2.3
21	2Z	174	VAL	2.3
33	2b	96	ARG	2.3
34	2c	173	VAL	2.3
40	1i	109	VAL	2.3
47	2p	79	VAL	2.3
10	2O	31	LYS	2.3
38	1g	84	ASN	2.3
38	2g	109	ASN	2.3
3	2D	210	GLY	2.3
34	1c	41	GLY	2.3
34	2c	9	GLY	2.3
38	1g	120	ILE	2.3
50	2s	12	ASP	2.3
50	2s	24	ALA	2.3
39	2h	24	THR	2.3
7	2H	164	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	2A	884	C	2.3
7	2H	167	GLU	2.3
20	2Y	55	TYR	2.3
32	1a	999	C	2.3
32	2a	1066	C	2.3
32	2a	1249	C	2.3
43	1l	60	LEU	2.3
47	2p	6	LEU	2.3
54	2w	42	C	2.3
1	2A	2169	A	2.2
32	1a	1447	A	2.2
32	2a	986	A	2.2
43	1l	23	LYS	2.2
51	2t	21	LYS	2.2
1	1A	2792	G	2.2
1	1A	1097	U	2.2
36	2e	85	GLY	2.2
56	1y	47	U	2.2
8	2I	59	ALA	2.2
48	1q	90	ILE	2.2
7	2H	90	LYS	2.2
7	2H	175	LYS	2.2
8	2I	9	LEU	2.2
9	2N	74	ARG	2.2
33	2b	149	LEU	2.2
34	2c	196	LEU	2.2
39	1h	112	LEU	2.2
39	2h	84	ARG	2.2
40	2i	4	TYR	2.2
41	2j	29	ARG	2.2
48	1q	89	LEU	2.2
31	29	24	TYR	2.2
54	2w	25	C	2.2
1	2A	887	A	2.2
26	14	50	VAL	2.2
34	1c	198	VAL	2.2
42	2k	80	VAL	2.2
53	2v	14	A	2.2
56	2y	59	U	2.2
1	2A	2157	G	2.2
1	2A	2792	G	2.2
11	1P	149	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
34	1c	8	ILE	2.2
7	2H	109	PHE	2.2
36	2e	28	PHE	2.2
47	1p	64	ALA	2.2
34	2c	15	THR	2.2
46	2o	68	ARG	2.2
22	20	62	LEU	2.2
47	2p	15	PRO	2.2
20	2Y	43	ASN	2.2
4	2E	75	VAL	2.2
5	2F	193	VAL	2.2
35	2d	198	VAL	2.2
32	2a	950	U	2.2
40	2i	70	LYS	2.2
51	1t	21	LYS	2.2
1	1A	2181	G	2.2
6	2G	2	PRO	2.2
7	2H	21	PRO	2.2
13	2R	29	LEU	2.2
8	2I	43	ASN	2.2
26	24	29	PRO	2.2
51	1t	43	LEU	2.2
34	2c	58	GLU	2.2
8	2I	96	ASP	2.2
40	2i	24	GLY	2.2
10	2O	7	TYR	2.2
12	2Q	18	LYS	2.2
14	2S	7	TYR	2.2
31	29	15	LYS	2.2
6	2G	160	VAL	2.2
39	2h	91	ARG	2.2
1	2A	899	A	2.2
8	1I	109	ILE	2.2
16	1U	69	CYS	2.2
32	1a	171	A	2.2
38	2g	39	ALA	2.2
35	2d	110	PHE	2.2
41	2j	92	THR	2.2
50	1s	40	ILE	2.2
33	2b	105	PHE	2.2
3	2D	155	LEU	2.2
28	26	9	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
35	2d	108	LEU	2.2
39	2h	89	PRO	2.2
40	2i	68	GLY	2.2
45	1n	14	PRO	2.2
1	1A	2133	G	2.2
1	2A	2151	G	2.2
6	2G	21	ARG	2.2
26	24	56	VAL	2.2
32	1a	1446	U	2.2
32	2a	1446	U	2.2
1	2A	2142	C	2.2
11	2P	68	GLN	2.2
56	1y	13	C	2.2
32	2a	1285	A	2.2
56	2y	58	A	2.2
18	2W	86	LEU	2.2
19	1X	70	LEU	2.2
40	1i	49	PRO	2.2
45	1n	51	GLY	2.2
49	2r	66	LEU	2.2
15	1T	115	ARG	2.2
31	29	19	ARG	2.2
33	2b	233	SER	2.2
35	1d	4	TYR	2.2
40	1i	114	TYR	2.2
48	2q	29	HIS	2.2
6	2G	15	VAL	2.2
48	1q	9	VAL	2.2
56	2y	45	U	2.2
8	2I	49	ALA	2.2
3	2D	50	THR	2.2
32	2a	1045	C	2.2
33	2b	200	ILE	2.2
34	2c	57	ILE	2.2
54	1w	41	C	2.2
38	2g	41	ARG	2.2
51	2t	86	ARG	2.2
4	1E	195	LEU	2.2
12	2Q	125	LEU	2.2
13	2R	10	LEU	2.2
32	1a	1286	A	2.2
41	1j	40	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
46	1o	31	LEU	2.2
46	1o	81	LEU	2.2
41	2j	13	HIS	2.1
35	2d	27	TYR	2.1
1	2A	2150	U	2.1
21	1Z	39	VAL	2.1
47	1p	48	TRP	2.1
32	2a	723	U	2.1
48	2q	85	VAL	2.1
21	2Z	4	ARG	2.1
43	2l	44	THR	2.1
46	1o	82	ILE	2.1
1	1A	2142	C	2.1
1	1A	2143	C	2.1
32	2a	970	C	2.1
21	2Z	150	LEU	2.1
51	2t	84	LEU	2.1
32	2a	1014	A	2.1
54	2w	23	A	2.1
42	2k	119	CYS	2.1
34	2c	23	TYR	2.1
35	2d	68	TYR	2.1
44	2m	71	ARG	2.1
45	2n	21	TYR	2.1
7	2H	17	VAL	2.1
8	2I	142	VAL	2.1
16	2U	90	VAL	2.1
23	2I	51	VAL	2.1
40	2i	112	LYS	2.1
5	2F	83	PHE	2.1
50	2s	10	PHE	2.1
56	2y	52	G	2.1
6	2G	139	LEU	2.1
10	1O	91	LEU	2.1
32	2a	1325	C	2.1
32	2a	1354	C	2.1
6	2G	181	ARG	2.1
38	2g	78	ARG	2.1
47	1p	29	ASP	2.1
51	1t	23	ARG	2.1
34	2c	120	VAL	2.1
35	2d	121	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
40	2i	45	ALA	2.1
40	2i	92	TYR	2.1
3	2D	40	THR	2.1
7	2H	8	PRO	2.1
33	2b	211	ILE	2.1
6	2G	141	PHE	2.1
1	1A	1176	G	2.1
1	1A	1092	C	2.1
1	1A	2896	C	2.1
32	2a	1217	C	2.1
32	2a	1254	C	2.1
35	2d	47	ARG	2.1
23	2l	29	GLY	2.1
34	2c	197	GLY	2.1
42	2k	49	GLY	2.1
32	2a	1447	A	2.1
1	1A	2118	U	2.1
5	2F	49	ALA	2.1
7	2H	146	ALA	2.1
33	1b	188	ALA	2.1
34	2c	71	ALA	2.1
15	1T	59	THR	2.1
23	2l	71	TYR	2.1
29	27	46	VAL	2.1
54	2w	45	U	2.1
39	1h	5	PRO	2.1
21	2Z	171	ILE	2.1
23	1l	7	ILE	2.1
7	2H	32	GLU	2.1
21	1Z	104	PHE	2.1
35	1d	101	LEU	2.1
44	2m	64	TRP	2.1
9	2N	83	LYS	2.1
41	2j	57	LYS	2.1
32	2a	1197	G	2.1
32	2a	1226	C	2.1
54	1w	48	C	2.1
56	2y	29	G	2.1
40	2i	73	GLN	2.1
45	2n	52	GLN	2.1
1	1A	2113	U	2.1
12	2Q	94	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
33	2b	171	ALA	2.1
33	2b	173	ALA	2.1
50	1s	75	ALA	2.1
41	2j	39	PRO	2.1
41	2j	41	PRO	2.1
42	1k	25	TYR	2.1
48	1q	96	GLU	2.1
15	1T	111	ARG	2.1
48	2q	32	TYR	2.1
15	2T	48	ILE	2.1
28	26	54	ILE	2.1
51	2t	100	ILE	2.1
14	1S	4	LEU	2.1
27	25	58	LEU	2.1
28	26	20	ASN	2.1
40	2i	6	GLY	2.1
1	1A	892	G	2.1
30	28	15	LYS	2.1
35	1d	189	PRO	2.1
41	1j	18	ALA	2.1
44	2m	80	ARG	2.1
54	2w	34	G	2.1
1	1A	1963	U	2.1
4	2E	104	VAL	2.1
9	2N	98	VAL	2.1
36	2e	100	VAL	2.1
36	2e	115	VAL	2.1
43	2l	61	THR	2.1
47	1p	38	TYR	2.1
21	2Z	137	ILE	2.1
48	2q	86	GLU	2.1
24	22	8	LYS	2.1
38	1g	32	ARG	2.1
51	2t	80	ARG	2.1
32	2a	1320	C	2.0
33	2b	34	ALA	2.0
34	1c	160	ALA	2.0
54	1w	4	C	2.0
1	2A	2172	U	2.0
32	2a	981	U	2.0
33	2b	184	VAL	2.0
39	1h	93	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
4	2E	81	ILE	2.0
8	2I	29	TYR	2.0
32	2a	1222	G	2.0
1	2A	2158	A	2.0
9	2N	68	GLU	2.0
26	24	45	GLY	2.0
32	1a	344	A	2.0
35	1d	69	GLY	2.0
35	2d	206	PHE	2.0
40	1i	59	PHE	2.0
40	1i	112	LYS	2.0
14	2S	23	ARG	2.0
45	1n	3	ARG	2.0
48	2q	30	PRO	2.0
50	2s	76	PRO	2.0
51	2t	59	ALA	2.0
8	2I	117	GLU	2.0
32	2a	1019	C	2.0
33	2b	229	VAL	2.0
35	2d	28	SER	2.0
6	2G	157	ILE	2.0
10	2O	114	ILE	2.0
15	2T	100	TYR	2.0
33	2b	127	ILE	2.0
43	2l	47	LYS	2.0
34	2c	205	GLY	2.0
37	2f	59	TYR	2.0
47	1p	25	ARG	2.0
49	1r	76	LEU	2.0
3	2D	15	PHE	2.0
1	2A	1445	A	2.0
1	2A	1847	A	2.0
54	2w	35	A	2.0
7	2H	29	PRO	2.0
42	2k	23	ALA	2.0
44	1m	107	ALA	2.0
49	1r	73	ALA	2.0
51	1t	66	ALA	2.0
8	2I	86	THR	2.0
17	2V	47	VAL	2.0
48	2q	35	VAL	2.0
32	1a	201	C	2.0

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Mol	Chain	Res	Type	RSRZ
32	1a	984	C	2.0
5	2F	32	LEU	2.0
8	2I	44	LEU	2.0
35	2d	186	LEU	2.0
39	1h	35	ILE	2.0
43	2l	70	ILE	2.0
48	2q	84	LEU	2.0
17	2V	81	TYR	2.0
33	2b	17	PHE	2.0
47	2p	39	TYR	2.0
1	2A	2134	A	2.0
1	2A	2148	G	2.0
2	2B	23	G	2.0
56	2y	53	G	2.0
33	2b	183	PRO	2.0
34	2c	7	PRO	2.0
34	2c	142	MET	2.0
48	2q	82	MET	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
56	PSU	2y	55	20/21	0.71	0.34	87,95,102,109	0
56	PSU	1y	55	20/21	0.74	0.28	83,88,100,106	0
56	7MG	2y	46	24/25	0.75	0.22	86,94,100,112	0
54	7MG	1w	46	24/25	0.76	0.20	77,86,96,115	0
54	7MG	2w	46	24/25	0.77	0.26	80,91,98,112	0
56	5MU	2y	54	21/22	0.78	0.36	88,92,99,117	0
56	PSU	2y	32	20/21	0.79	0.24	71,82,95,95	0
56	5MU	1y	54	21/22	0.79	0.26	78,83,92,101	0
56	4SU	2y	8	20/21	0.80	0.15	88,92,98,104	0
54	4SU	2w	8	20/21	0.81	0.26	87,95,103,113	0
54	PSU	2w	55	20/21	0.81	0.28	81,87,92,98	0
56	4SU	1y	8	20/21	0.84	0.16	83,87,95,95	0
56	7MG	1y	46	24/25	0.85	0.21	80,89,98,108	0
54	PSU	1w	55	20/21	0.86	0.26	63,81,85,87	0
56	MIA	2y	37	22/30	0.86	0.25	76,84,93,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	4SU	2x	8	20/21	0.86	0.15	74,79,83,91	0
54	MIA	2w	37	25/30	0.87	0.30	78,85,89,102	0
32	2MG	2a	1207	24/25	0.87	0.18	79,87,95,98	0
54	PSU	2w	32	20/21	0.87	0.38	82,88,94,98	0
54	5MU	2w	54	21/22	0.88	0.19	78,82,90,92	0
43	0TD	1l	92	10/11	0.88	0.19	44,53,57,69	0
32	PSU	2a	516	20/21	0.88	0.19	79,81,87,89	0
32	M2G	2a	966	25/26	0.88	0.24	60,70,84,89	0
43	0TD	2l	92	10/11	0.89	0.25	67,69,75,87	0
55	5MU	2x	54	21/22	0.89	0.20	77,81,89,99	0
56	PSU	1y	39	20/21	0.90	0.17	70,76,82,83	0
56	MIA	1y	37	22/30	0.90	0.17	65,74,81,86	0
32	5MC	2a	967	21/22	0.90	0.21	68,73,80,84	0
56	PSU	2y	39	20/21	0.90	0.22	78,81,93,96	0
54	4SU	1w	8	20/21	0.90	0.20	78,82,90,94	0
55	PSU	2x	55	20/21	0.90	0.17	75,81,83,89	0
54	PSU	2w	39	20/21	0.91	0.45	79,84,88,89	0
54	PSU	1w	32	20/21	0.92	0.32	68,73,86,90	0
1	5MU	2A	1915	21/22	0.92	0.13	71,75,81,92	0
32	5MC	2a	1404	21/22	0.92	0.23	59,64,67,71	0
56	PSU	1y	32	20/21	0.93	0.21	73,76,81,82	0
54	MIA	1w	37	29/30	0.93	0.28	55,64,74,79	0
54	PSU	1w	39	20/21	0.94	0.27	63,74,77,81	0
1	PSU	2A	1911	20/21	0.94	0.16	54,63,72,74	0
32	MA6	2a	1519	24/25	0.94	0.26	51,66,71,73	0
1	PSU	2A	1917	20/21	0.94	0.16	62,70,76,83	0
55	PSU	1x	55	20/21	0.94	0.17	46,61,70,71	0
32	4OC	2a	1402	22/23	0.94	0.15	58,66,73,76	0
32	UR3	2a	1498	21/22	0.95	0.21	60,63,70,74	0
1	5MU	1A	1915	21/22	0.95	0.16	40,55,60,62	0
1	OMC	2A	1920	21/22	0.95	0.17	59,64,68,69	0
32	PSU	1a	516	20/21	0.95	0.15	58,62,67,69	0
55	5MC	2x	32	21/22	0.95	0.18	68,74,78,81	0
55	5MU	1x	54	21/22	0.95	0.14	59,65,71,77	0
1	PSU	1A	1917	20/21	0.95	0.18	39,48,54,59	0
32	7MG	2a	527	24/25	0.95	0.18	60,67,73,83	0
54	5MU	1w	54	21/22	0.95	0.17	61,72,78,81	0
32	MA6	2a	1518	24/25	0.96	0.20	52,67,72,73	0
32	5MC	1a	967	21/22	0.96	0.21	50,56,63,64	0
1	5MC	2A	1962	21/22	0.96	0.18	42,50,58,66	0
32	2MG	1a	1207	24/25	0.96	0.15	56,65,68,72	0
32	7MG	1a	527	24/25	0.96	0.17	40,48,52,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	4SU	1x	8	20/21	0.96	0.15	55,61,65,65	0
32	5MC	2a	1400	21/22	0.96	0.26	71,74,78,82	0
32	4OC	1a	1402	22/23	0.96	0.18	39,48,54,54	0
1	PSU	2A	2605	20/21	0.96	0.18	33,40,43,47	0
32	M2G	1a	966	25/26	0.96	0.19	47,54,60,64	0
32	5MC	2a	1407	21/22	0.96	0.20	55,59,64,65	0
1	5MC	2A	1942	21/22	0.96	0.19	50,56,64,64	0
1	OMG	2A	2251	24/25	0.97	0.19	39,42,46,48	0
1	OMU	2A	2552	21/22	0.97	0.22	39,44,49,59	0
32	MA6	1a	1519	24/25	0.97	0.20	35,41,45,52	0
1	5MC	1A	1942	21/22	0.97	0.17	33,40,46,48	0
55	5MC	1x	32	21/22	0.97	0.19	48,53,59,68	0
55	31H	1x	76	32/33	0.97	0.21	22,29,37,42	10
55	31H	2x	76	32/33	0.97	0.22	40,48,54,68	0
1	OMC	1A	1920	21/22	0.98	0.19	38,45,50,52	0
1	2MA	1A	2503	23/24	0.98	0.20	14,20,24,26	0
1	2MA	2A	2503	23/24	0.98	0.21	29,37,42,45	0
32	5MC	1a	1404	21/22	0.98	0.19	38,42,46,50	0
1	OMU	1A	2552	21/22	0.98	0.22	23,30,35,38	0
32	5MC	1a	1407	21/22	0.98	0.18	33,40,45,49	0
1	PSU	1A	1911	20/21	0.98	0.18	36,45,52,52	0
32	UR3	1a	1498	21/22	0.98	0.18	38,41,43,47	0
1	5MC	1A	1962	21/22	0.98	0.18	27,34,40,50	0
1	5MU	2A	1939	21/22	0.98	0.20	35,39,47,48	0
1	OMG	1A	2251	24/25	0.98	0.20	22,26,30,32	0
32	5MC	1a	1400	21/22	0.98	0.18	43,51,56,63	0
1	PSU	1A	2605	20/21	0.99	0.19	21,26,30,32	0
1	5MU	1A	1939	21/22	0.99	0.21	22,28,33,34	0
32	MA6	1a	1518	24/25	0.99	0.21	31,42,46,48	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(\AA^2)	Q<0.9
57	MG	1A	3932	1/1	0.11	0.16	70,70,70,70	0
57	MG	1Y	203	1/1	0.22	0.20	84,84,84,84	0
57	MG	1A	3931	1/1	0.23	0.20	72,72,72,72	0
57	MG	1A	3959	1/1	0.28	0.14	48,48,48,48	0
57	MG	1a	1642	1/1	0.30	0.20	78,78,78,78	0
57	MG	2A	3556	1/1	0.36	0.49	80,80,80,80	0
57	MG	1A	3401	1/1	0.37	0.39	77,77,77,77	0
57	MG	2A	3251	1/1	0.39	0.14	71,71,71,71	0
57	MG	2a	1658	1/1	0.40	0.16	78,78,78,78	0
57	MG	1a	1715	1/1	0.43	0.27	59,59,59,59	0
57	MG	1A	4014	1/1	0.44	0.10	69,69,69,69	0
57	MG	2a	1753	1/1	0.45	0.24	71,71,71,71	0
57	MG	2a	1616	1/1	0.46	0.43	80,80,80,80	0
57	MG	2A	3341	1/1	0.48	0.30	63,63,63,63	0
57	MG	1A	3953	1/1	0.49	0.09	50,50,50,50	0
57	MG	1A	3754	1/1	0.50	0.10	59,59,59,59	0
57	MG	2A	3576	1/1	0.52	0.08	70,70,70,70	0
57	MG	1A	3935	1/1	0.52	0.11	68,68,68,68	0
57	MG	2A	3551	1/1	0.52	0.26	79,79,79,79	0
57	MG	1A	4049	1/1	0.52	0.10	59,59,59,59	0
59	ZN	24	501	1/1	0.52	0.13	135,135,135,135	0
57	MG	1A	4042	1/1	0.53	0.25	60,60,60,60	0
57	MG	1A	3490	1/1	0.53	0.27	63,63,63,63	0
57	MG	2A	3452	1/1	0.55	0.20	73,73,73,73	0
57	MG	1A	4006	1/1	0.55	0.14	46,46,46,46	0
57	MG	1A	3853	1/1	0.57	0.11	55,55,55,55	0
57	MG	2a	1663	1/1	0.57	0.27	74,74,74,74	0
57	MG	2A	3579	1/1	0.58	0.16	70,70,70,70	0
57	MG	1A	3716	1/1	0.58	0.16	37,37,37,37	0
57	MG	2A	3687	1/1	0.59	0.09	69,69,69,69	0
57	MG	1A	3604	1/1	0.59	0.23	47,47,47,47	0
57	MG	1A	4033	1/1	0.59	0.12	80,80,80,80	0
57	MG	2A	3560	1/1	0.59	0.20	64,64,64,64	0
57	MG	2A	3486	1/1	0.59	0.17	54,54,54,54	0
57	MG	2A	3533	1/1	0.59	0.15	72,72,72,72	0
57	MG	2A	3722	1/1	0.60	0.19	78,78,78,78	0
57	MG	1A	4003	1/1	0.60	0.19	74,74,74,74	0
57	MG	1A	3972	1/1	0.61	0.12	40,40,40,40	0
57	MG	2a	1646	1/1	0.61	0.17	76,76,76,76	0
57	MG	1a	1784	1/1	0.61	0.19	69,69,69,69	0
57	MG	2A	3544	1/1	0.62	0.60	68,68,68,68	0
57	MG	1A	3930	1/1	0.62	0.13	72,72,72,72	0
57	MG	2A	3555	1/1	0.62	0.31	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	4002	1/1	0.62	0.11	86,86,86,86	0
57	MG	1a	1675	1/1	0.62	0.13	58,58,58,58	0
57	MG	1A	3679	1/1	0.62	0.24	31,31,31,31	0
57	MG	1A	3967	1/1	0.62	0.14	49,49,49,49	0
57	MG	2A	3605	1/1	0.62	0.14	70,70,70,70	0
57	MG	2A	3607	1/1	0.63	0.16	60,60,60,60	0
57	MG	2A	3648	1/1	0.63	0.35	76,76,76,76	0
57	MG	1a	1629	1/1	0.63	0.13	51,51,51,51	0
57	MG	1A	3529	1/1	0.63	0.26	66,66,66,66	0
57	MG	1A	3297	1/1	0.63	0.14	59,59,59,59	0
57	MG	1B	212	1/1	0.64	0.10	59,59,59,59	0
57	MG	1A	3553	1/1	0.64	0.42	62,62,62,62	0
57	MG	2a	1626	1/1	0.65	0.13	71,71,71,71	0
57	MG	2a	1640	1/1	0.65	0.29	76,76,76,76	0
57	MG	1A	3973	1/1	0.65	0.12	56,56,56,56	0
57	MG	2A	3656	1/1	0.65	0.10	64,64,64,64	0
57	MG	2A	3259	1/1	0.65	0.26	71,71,71,71	0
57	MG	2A	3168	1/1	0.65	0.20	67,67,67,67	0
57	MG	2v	101	1/1	0.65	0.19	77,77,77,77	0
57	MG	2A	3615	1/1	0.65	0.16	74,74,74,74	0
57	MG	2A	3466	1/1	0.66	0.11	54,54,54,54	0
57	MG	2A	3696	1/1	0.66	0.12	45,45,45,45	0
57	MG	1A	3986	1/1	0.66	0.12	60,60,60,60	0
57	MG	1B	234	1/1	0.66	0.14	67,67,67,67	0
57	MG	1b	302	1/1	0.66	0.11	80,80,80,80	0
57	MG	1A	3338	1/1	0.66	0.36	51,51,51,51	0
57	MG	1A	3917	1/1	0.67	0.22	56,56,56,56	0
57	MG	2a	1742	1/1	0.67	0.32	65,65,65,65	0
57	MG	2A	3481	1/1	0.67	0.15	63,63,63,63	0
57	MG	1A	3538	1/1	0.67	0.16	65,65,65,65	0
57	MG	1U	209	1/1	0.67	0.20	53,53,53,53	0
57	MG	2a	1621	1/1	0.68	0.14	78,78,78,78	0
57	MG	1a	1788	1/1	0.68	0.31	85,85,85,85	0
57	MG	2a	1629	1/1	0.68	0.18	74,74,74,74	0
57	MG	1a	1678	1/1	0.68	0.16	64,64,64,64	0
57	MG	2A	3355	1/1	0.68	0.21	68,68,68,68	0
57	MG	2A	3100	1/1	0.68	0.14	60,60,60,60	0
57	MG	2A	3719	1/1	0.68	0.20	62,62,62,62	0
57	MG	1E	314	1/1	0.68	0.21	62,62,62,62	0
57	MG	2B	206	1/1	0.68	0.20	68,68,68,68	0
57	MG	28	103	1/1	0.68	0.17	75,75,75,75	0
57	MG	1A	3692	1/1	0.68	0.24	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3409	1/1	0.69	0.13	51,51,51,51	0
57	MG	1w	101	1/1	0.69	0.17	76,76,76,76	0
57	MG	2a	1722	1/1	0.69	0.17	56,56,56,56	0
57	MG	2A	3188	1/1	0.69	0.20	52,52,52,52	0
57	MG	1A	4031	1/1	0.69	0.12	58,58,58,58	0
57	MG	2A	3552	1/1	0.69	0.20	79,79,79,79	0
57	MG	2A	3684	1/1	0.69	0.09	55,55,55,55	0
57	MG	2A	3404	1/1	0.70	0.10	67,67,67,67	0
57	MG	1f	201	1/1	0.70	0.21	55,55,55,55	0
57	MG	2A	3293	1/1	0.70	0.28	53,53,53,53	0
57	MG	1a	1721	1/1	0.70	0.19	81,81,81,81	0
57	MG	1A	4063	1/1	0.70	0.23	70,70,70,70	0
57	MG	2A	3446	1/1	0.71	0.30	53,53,53,53	0
57	MG	2A	3149	1/1	0.71	0.16	53,53,53,53	0
57	MG	2A	3601	1/1	0.71	0.19	72,72,72,72	0
57	MG	1A	3761	1/1	0.71	0.19	60,60,60,60	0
57	MG	18	3405	1/1	0.71	0.25	48,48,48,48	0
57	MG	1a	1676	1/1	0.71	0.30	64,64,64,64	0
57	MG	1A	3232	1/1	0.71	0.15	62,62,62,62	0
57	MG	1A	4101	1/1	0.72	0.20	43,43,43,43	0
57	MG	1A	3952	1/1	0.72	0.11	51,51,51,51	0
57	MG	1a	1615	1/1	0.72	0.15	58,58,58,58	0
57	MG	2A	3265	1/1	0.72	0.15	56,56,56,56	0
57	MG	2A	3575	1/1	0.72	0.12	74,74,74,74	0
57	MG	2A	3005	1/1	0.72	0.21	62,62,62,62	0
57	MG	2a	1687	1/1	0.72	0.14	67,67,67,67	0
57	MG	1A	3459	1/1	0.72	0.16	70,70,70,70	0
57	MG	2A	3496	1/1	0.72	0.12	66,66,66,66	0
57	MG	1A	3778	1/1	0.72	0.19	34,34,34,34	0
57	MG	2A	3370	1/1	0.72	0.26	60,60,60,60	0
57	MG	1A	3811	1/1	0.72	0.17	58,58,58,58	0
57	MG	1a	1760	1/1	0.73	0.09	80,80,80,80	0
57	MG	2A	3039	1/1	0.73	0.24	66,66,66,66	0
57	MG	2A	3075	1/1	0.73	0.23	65,65,65,65	0
57	MG	1a	1781	1/1	0.73	0.13	71,71,71,71	0
57	MG	1A	3728	1/1	0.73	0.08	63,63,63,63	0
57	MG	2a	1693	1/1	0.73	0.20	78,78,78,78	0
57	MG	2a	1714	1/1	0.73	0.15	74,74,74,74	0
57	MG	1A	3508	1/1	0.73	0.19	53,53,53,53	0
57	MG	1E	301	1/1	0.73	0.21	32,32,32,32	0
57	MG	2A	3232	1/1	0.73	0.17	62,62,62,62	0
57	MG	1A	3057	1/1	0.73	0.22	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3722	1/1	0.73	0.17	50,50,50,50	0
57	MG	2A	3640	1/1	0.74	0.14	66,66,66,66	0
57	MG	2A	3243	1/1	0.74	0.23	52,52,52,52	0
57	MG	2a	1644	1/1	0.74	0.21	61,61,61,61	0
57	MG	1a	1717	1/1	0.74	0.12	66,66,66,66	0
57	MG	2A	3415	1/1	0.74	0.15	37,37,37,37	0
57	MG	2A	3442	1/1	0.74	0.17	69,69,69,69	0
57	MG	1E	303	1/1	0.74	0.46	44,44,44,44	0
57	MG	1A	3408	1/1	0.74	0.20	48,48,48,48	0
57	MG	2A	3266	1/1	0.74	0.10	59,59,59,59	0
57	MG	1A	3876	1/1	0.74	0.35	57,57,57,57	0
57	MG	1y	101	1/1	0.74	0.12	68,68,68,68	0
57	MG	1A	3934	1/1	0.74	0.10	32,32,32,32	0
57	MG	2A	3028	1/1	0.74	0.17	59,59,59,59	0
57	MG	2A	3378	1/1	0.74	0.17	63,63,63,63	0
57	MG	1a	1693	1/1	0.75	0.15	69,69,69,69	0
57	MG	1A	3703	1/1	0.75	0.18	68,68,68,68	0
57	MG	1B	230	1/1	0.75	0.12	75,75,75,75	0
57	MG	1a	1660	1/1	0.75	0.10	65,65,65,65	0
57	MG	1w	105	1/1	0.75	0.10	70,70,70,70	0
57	MG	1x	114	1/1	0.75	0.16	70,70,70,70	0
57	MG	2A	3524	1/1	0.75	0.17	72,72,72,72	0
57	MG	1a	1758	1/1	0.75	0.45	69,69,69,69	0
57	MG	1A	3255	1/1	0.75	0.32	61,61,61,61	0
57	MG	1A	3819	1/1	0.75	0.20	58,58,58,58	0
57	MG	2a	1780	1/1	0.75	0.11	67,67,67,67	0
57	MG	1A	3489	1/1	0.75	0.17	61,61,61,61	0
57	MG	2A	3445	1/1	0.75	0.19	48,48,48,48	0
57	MG	1A	4046	1/1	0.76	0.33	53,53,53,53	0
57	MG	1A	4015	1/1	0.76	0.10	59,59,59,59	0
57	MG	2A	3052	1/1	0.76	0.18	66,66,66,66	0
57	MG	2A	3053	1/1	0.76	0.26	74,74,74,74	0
57	MG	2A	3276	1/1	0.76	0.10	59,59,59,59	0
57	MG	1a	1734	1/1	0.76	0.15	54,54,54,54	0
57	MG	1l	201	1/1	0.76	0.24	65,65,65,65	0
57	MG	2A	3518	1/1	0.76	0.15	54,54,54,54	0
57	MG	1a	1741	1/1	0.76	0.13	79,79,79,79	0
57	MG	2A	3368	1/1	0.76	0.28	63,63,63,63	0
57	MG	1A	3977	1/1	0.76	0.14	53,53,53,53	0
57	MG	1A	3169	1/1	0.76	0.26	62,62,62,62	0
57	MG	2A	3692	1/1	0.76	0.24	71,71,71,71	0
57	MG	2A	3205	1/1	0.76	0.15	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3226	1/1	0.76	0.32	74,74,74,74	0
57	MG	2a	1762	1/1	0.76	0.30	69,69,69,69	0
57	MG	1A	3756	1/1	0.76	0.21	63,63,63,63	0
57	MG	1O	201	1/1	0.76	0.43	72,72,72,72	0
57	MG	2A	3569	1/1	0.76	0.14	61,61,61,61	0
57	MG	1A	3016	1/1	0.77	0.29	56,56,56,56	0
57	MG	1a	1786	1/1	0.77	0.12	56,56,56,56	0
57	MG	1A	3768	1/1	0.77	0.19	49,49,49,49	0
57	MG	1a	1669	1/1	0.77	0.20	57,57,57,57	0
57	MG	2A	3047	1/1	0.77	0.18	69,69,69,69	0
57	MG	1A	3399	1/1	0.77	0.18	51,51,51,51	0
57	MG	1A	4065	1/1	0.77	0.22	50,50,50,50	0
57	MG	2A	3065	1/1	0.77	0.11	65,65,65,65	0
57	MG	2a	1604	1/1	0.77	0.12	59,59,59,59	0
57	MG	1A	3993	1/1	0.77	0.10	64,64,64,64	0
57	MG	2A	3638	1/1	0.77	0.14	67,67,67,67	0
57	MG	1a	1683	1/1	0.77	0.13	72,72,72,72	0
57	MG	1B	204	1/1	0.77	0.35	63,63,63,63	0
57	MG	2A	3158	1/1	0.77	0.12	67,67,67,67	0
57	MG	1A	4038	1/1	0.78	0.36	57,57,57,57	0
57	MG	2B	203	1/1	0.78	0.20	62,62,62,62	0
57	MG	1A	3093	1/1	0.78	0.16	58,58,58,58	0
57	MG	2A	3170	1/1	0.78	0.16	57,57,57,57	0
57	MG	2A	3175	1/1	0.78	0.18	71,71,71,71	0
57	MG	1a	1779	1/1	0.78	0.15	55,55,55,55	0
57	MG	1y	102	1/1	0.78	0.15	88,88,88,88	0
57	MG	2A	3209	1/1	0.78	0.16	59,59,59,59	0
57	MG	2A	3210	1/1	0.78	0.15	69,69,69,69	0
57	MG	2A	3581	1/1	0.78	0.16	63,63,63,63	0
57	MG	2A	3223	1/1	0.78	0.14	72,72,72,72	0
57	MG	1A	3330	1/1	0.78	0.38	52,52,52,52	0
57	MG	1B	224	1/1	0.78	0.24	70,70,70,70	0
57	MG	1A	3208	1/1	0.78	0.24	64,64,64,64	0
57	MG	1A	4050	1/1	0.78	0.11	57,57,57,57	0
57	MG	1a	1811	1/1	0.78	0.11	67,67,67,67	0
57	MG	1a	1817	1/1	0.78	0.10	58,58,58,58	0
57	MG	1A	4056	1/1	0.78	0.18	44,44,44,44	0
57	MG	2a	1727	1/1	0.78	0.17	71,71,71,71	0
57	MG	2A	3663	1/1	0.78	0.15	58,58,58,58	0
57	MG	1a	1651	1/1	0.78	0.15	66,66,66,66	0
57	MG	1A	3519	1/1	0.78	0.19	52,52,52,52	0
57	MG	2A	3313	1/1	0.78	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
57	MG	2A	3550	1/1	0.78	0.14	63,63,63,63	0
57	MG	1A	3365	1/1	0.78	0.30	60,60,60,60	0
57	MG	1A	3966	1/1	0.79	0.15	52,52,52,52	0
57	MG	2A	3703	1/1	0.79	0.21	67,67,67,67	0
57	MG	2A	3711	1/1	0.79	0.13	61,61,61,61	0
57	MG	2A	3537	1/1	0.79	0.13	60,60,60,60	0
57	MG	2A	3309	1/1	0.79	0.20	56,56,56,56	0
57	MG	2A	3102	1/1	0.79	0.11	55,55,55,55	0
57	MG	1A	3476	1/1	0.79	0.26	70,70,70,70	0
57	MG	2B	217	1/1	0.79	0.11	76,76,76,76	0
57	MG	2A	3350	1/1	0.79	0.11	50,50,50,50	0
57	MG	1A	3298	1/1	0.79	0.27	51,51,51,51	0
57	MG	1x	108	1/1	0.79	0.17	68,68,68,68	0
57	MG	1x	113	1/1	0.79	0.14	72,72,72,72	0
57	MG	1A	3438	1/1	0.79	0.15	43,43,43,43	0
57	MG	2A	3396	1/1	0.79	0.19	38,38,38,38	0
57	MG	1A	4061	1/1	0.79	0.13	55,55,55,55	0
57	MG	1A	3268	1/1	0.79	0.16	57,57,57,57	0
57	MG	2A	3001	1/1	0.79	0.29	57,57,57,57	0
57	MG	2a	1650	1/1	0.79	0.12	74,74,74,74	0
57	MG	2A	3434	1/1	0.79	0.12	36,36,36,36	0
57	MG	1A	3509	1/1	0.79	0.16	44,44,44,44	0
57	MG	2a	1680	1/1	0.79	0.11	62,62,62,62	0
57	MG	1A	4098	1/1	0.79	0.13	54,54,54,54	0
57	MG	2a	1692	1/1	0.79	0.17	74,74,74,74	0
57	MG	1A	3466	1/1	0.79	0.29	49,49,49,49	0
57	MG	1B	203	1/1	0.79	0.18	31,31,31,31	0
57	MG	2a	1717	1/1	0.79	0.15	75,75,75,75	0
57	MG	2A	3048	1/1	0.79	0.15	63,63,63,63	0
57	MG	13	103	1/1	0.79	0.20	57,57,57,57	0
57	MG	1a	1698	1/1	0.79	0.30	65,65,65,65	0
57	MG	2A	3658	1/1	0.79	0.05	75,75,75,75	0
57	MG	1A	3525	1/1	0.79	0.18	49,49,49,49	0
57	MG	1a	1610	1/1	0.79	0.25	57,57,57,57	0
57	MG	2A	3095	1/1	0.79	0.23	61,61,61,61	0
57	MG	2A	3532	1/1	0.79	0.12	78,78,78,78	0
57	MG	2A	3562	1/1	0.80	0.13	46,46,46,46	0
57	MG	2A	3422	1/1	0.80	0.11	62,62,62,62	0
57	MG	1m	3001	1/1	0.80	0.11	57,57,57,57	0
57	MG	1A	3957	1/1	0.80	0.09	62,62,62,62	0
57	MG	1A	3342	1/1	0.80	0.36	62,62,62,62	0
57	MG	1A	3961	1/1	0.80	0.06	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2a	1622	1/1	0.80	0.19	68,68,68,68	0
57	MG	2A	3582	1/1	0.80	0.14	75,75,75,75	0
57	MG	1A	3183	1/1	0.80	0.10	70,70,70,70	0
57	MG	1A	3202	1/1	0.80	0.12	48,48,48,48	0
57	MG	1A	4030	1/1	0.80	0.10	61,61,61,61	0
57	MG	1F	308	1/1	0.80	0.33	49,49,49,49	0
57	MG	2A	3635	1/1	0.80	0.32	55,55,55,55	0
57	MG	1A	4095	1/1	0.80	0.29	66,66,66,66	0
57	MG	1O	204	1/1	0.80	0.20	64,64,64,64	0
57	MG	2A	3198	1/1	0.80	0.15	68,68,68,68	0
57	MG	2a	1681	1/1	0.80	0.16	68,68,68,68	0
57	MG	2A	3650	1/1	0.80	0.07	52,52,52,52	0
57	MG	2A	3356	1/1	0.80	0.11	76,76,76,76	0
57	MG	1A	3591	1/1	0.80	0.33	57,57,57,57	0
57	MG	2a	1702	1/1	0.80	0.18	57,57,57,57	0
57	MG	2a	1703	1/1	0.80	0.19	65,65,65,65	0
57	MG	1a	1691	1/1	0.80	0.19	72,72,72,72	0
57	MG	2A	3540	1/1	0.80	0.12	66,66,66,66	0
57	MG	2A	3543	1/1	0.80	0.21	62,62,62,62	0
57	MG	2A	3371	1/1	0.80	0.37	59,59,59,59	0
57	MG	2A	3372	1/1	0.80	0.20	54,54,54,54	0
57	MG	1a	1816	1/1	0.80	0.06	47,47,47,47	0
57	MG	1A	3092	1/1	0.80	0.15	59,59,59,59	0
57	MG	1A	3655	1/1	0.80	0.20	33,33,33,33	0
57	MG	2a	1784	1/1	0.80	0.24	71,71,71,71	0
57	MG	1A	3869	1/1	0.80	0.13	48,48,48,48	0
59	ZN	14	102	1/1	0.80	0.05	97,97,97,97	0
57	MG	1A	3295	1/1	0.80	0.17	45,45,45,45	0
57	MG	2a	1620	1/1	0.81	0.11	79,79,79,79	0
57	MG	1A	4019	1/1	0.81	0.20	35,35,35,35	0
57	MG	2A	3583	1/1	0.81	0.22	55,55,55,55	0
57	MG	2A	3160	1/1	0.81	0.13	59,59,59,59	0
57	MG	2A	3484	1/1	0.81	0.15	35,35,35,35	0
57	MG	2a	1636	1/1	0.81	0.07	81,81,81,81	0
57	MG	2A	3004	1/1	0.81	0.28	68,68,68,68	0
57	MG	1B	207	1/1	0.81	0.23	62,62,62,62	0
57	MG	2A	3632	1/1	0.81	0.10	64,64,64,64	0
57	MG	2a	1649	1/1	0.81	0.19	66,66,66,66	0
57	MG	2A	3506	1/1	0.81	0.16	46,46,46,46	0
57	MG	1A	3191	1/1	0.81	0.24	51,51,51,51	0
57	MG	1A	3496	1/1	0.81	0.11	43,43,43,43	0
57	MG	2A	3040	1/1	0.81	0.12	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3203	1/1	0.81	0.21	63,63,63,63	0
57	MG	1A	3673	1/1	0.81	0.14	49,49,49,49	0
57	MG	1A	3235	1/1	0.81	0.15	63,63,63,63	0
57	MG	2A	3050	1/1	0.81	0.14	56,56,56,56	0
57	MG	1A	3481	1/1	0.81	0.20	50,50,50,50	0
57	MG	1A	4045	1/1	0.81	0.20	56,56,56,56	0
57	MG	1x	102	1/1	0.81	0.17	33,33,33,33	0
57	MG	2A	3407	1/1	0.81	0.13	69,69,69,69	0
57	MG	1a	1692	1/1	0.81	0.13	74,74,74,74	0
57	MG	1A	3562	1/1	0.81	0.10	62,62,62,62	0
57	MG	1A	3460	1/1	0.81	0.69	55,55,55,55	0
57	MG	2A	3260	1/1	0.81	0.12	61,61,61,61	0
57	MG	2A	3563	1/1	0.81	0.11	61,61,61,61	0
57	MG	1a	1791	1/1	0.81	0.17	56,56,56,56	0
57	MG	2A	3121	1/1	0.81	0.28	67,67,67,67	0
57	MG	1a	1650	1/1	0.81	0.42	64,64,64,64	0
57	MG	2x	102	1/1	0.81	0.17	77,77,77,77	0
57	MG	2x	103	1/1	0.81	0.17	66,66,66,66	0
57	MG	2A	3449	1/1	0.81	0.14	48,48,48,48	0
57	MG	2A	3286	1/1	0.81	0.26	48,48,48,48	0
57	MG	1A	4025	1/1	0.82	0.14	48,48,48,48	0
57	MG	2A	3021	1/1	0.82	0.12	70,70,70,70	0
57	MG	1a	1771	1/1	0.82	0.15	56,56,56,56	0
57	MG	1A	3724	1/1	0.82	0.33	64,64,64,64	0
57	MG	2A	3521	1/1	0.82	0.14	45,45,45,45	0
57	MG	1a	1637	1/1	0.82	0.18	76,76,76,76	0
57	MG	2B	201	1/1	0.82	0.16	64,64,64,64	0
57	MG	1A	3061	1/1	0.82	0.26	50,50,50,50	0
57	MG	2A	3269	1/1	0.82	0.13	65,65,65,65	0
57	MG	2A	3535	1/1	0.82	0.09	59,59,59,59	0
57	MG	2F	301	1/1	0.82	0.20	54,54,54,54	0
57	MG	28	102	1/1	0.82	0.27	59,59,59,59	0
57	MG	1A	3420	1/1	0.82	0.17	41,41,41,41	0
57	MG	2A	3284	1/1	0.82	0.26	52,52,52,52	0
57	MG	2A	3542	1/1	0.82	0.22	69,69,69,69	0
57	MG	1A	3924	1/1	0.82	0.21	30,30,30,30	0
57	MG	1A	3548	1/1	0.82	0.19	52,52,52,52	0
57	MG	2A	3304	1/1	0.82	0.34	70,70,70,70	0
57	MG	1a	1809	1/1	0.82	0.14	63,63,63,63	0
57	MG	2a	1627	1/1	0.82	0.19	59,59,59,59	0
57	MG	2A	3064	1/1	0.82	0.12	59,59,59,59	0
57	MG	1A	3090	1/1	0.82	0.14	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3074	1/1	0.82	0.17	55,55,55,55	0
57	MG	1a	1813	1/1	0.82	0.08	68,68,68,68	0
57	MG	1A	3555	1/1	0.82	0.28	59,59,59,59	0
57	MG	1A	3212	1/1	0.82	0.31	42,42,42,42	0
57	MG	1A	3997	1/1	0.82	0.14	38,38,38,38	0
57	MG	2a	1657	1/1	0.82	0.14	65,65,65,65	0
57	MG	2A	3103	1/1	0.82	0.13	64,64,64,64	0
57	MG	1A	3163	1/1	0.82	0.17	50,50,50,50	0
57	MG	2a	1672	1/1	0.82	0.10	70,70,70,70	0
57	MG	1A	4058	1/1	0.82	0.19	44,44,44,44	0
57	MG	1A	3946	1/1	0.82	0.07	53,53,53,53	0
57	MG	1t	201	1/1	0.82	0.10	53,53,53,53	0
57	MG	1A	3719	1/1	0.82	0.16	46,46,46,46	0
57	MG	1w	103	1/1	0.82	0.10	63,63,63,63	0
57	MG	1w	104	1/1	0.82	0.18	69,69,69,69	0
57	MG	2A	3187	1/1	0.82	0.16	56,56,56,56	0
57	MG	2A	3426	1/1	0.82	0.10	48,48,48,48	0
57	MG	2A	3628	1/1	0.82	0.13	66,66,66,66	0
57	MG	1A	3837	1/1	0.82	0.19	52,52,52,52	0
57	MG	1a	1708	1/1	0.82	0.09	58,58,58,58	0
57	MG	1a	1713	1/1	0.82	0.12	57,57,57,57	0
57	MG	1A	4088	1/1	0.82	0.17	64,64,64,64	0
57	MG	1Z	3702	1/1	0.82	0.17	70,70,70,70	0
57	MG	1A	3847	1/1	0.82	0.27	58,58,58,58	0
57	MG	2A	3651	1/1	0.82	0.17	57,57,57,57	0
57	MG	2A	3455	1/1	0.82	0.13	62,62,62,62	0
57	MG	1A	3597	1/1	0.82	0.10	35,35,35,35	0
57	MG	2A	3470	1/1	0.82	0.20	62,62,62,62	0
57	MG	1a	1605	1/1	0.82	0.11	59,59,59,59	0
57	MG	1A	4100	1/1	0.82	0.19	62,62,62,62	0
57	MG	25	101	1/1	0.83	0.15	59,59,59,59	0
57	MG	26	101	1/1	0.83	0.16	61,61,61,61	0
57	MG	1a	1763	1/1	0.83	0.10	70,70,70,70	0
57	MG	1a	1769	1/1	0.83	0.09	57,57,57,57	0
57	MG	2a	1602	1/1	0.83	0.08	71,71,71,71	0
57	MG	2a	1603	1/1	0.83	0.13	65,65,65,65	0
57	MG	1a	1640	1/1	0.83	0.07	61,61,61,61	0
57	MG	2A	3212	1/1	0.83	0.20	66,66,66,66	0
57	MG	2A	3214	1/1	0.83	0.18	69,69,69,69	0
57	MG	1A	4044	1/1	0.83	0.10	53,53,53,53	0
57	MG	1A	3062	1/1	0.83	0.25	48,48,48,48	0
57	MG	1A	3731	1/1	0.83	0.15	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1a	1659	1/1	0.83	0.11	74,74,74,74	0
57	MG	1A	3277	1/1	0.83	0.35	35,35,35,35	0
57	MG	2A	3254	1/1	0.83	0.20	48,48,48,48	0
57	MG	2a	1637	1/1	0.83	0.12	73,73,73,73	0
57	MG	1A	3467	1/1	0.83	0.14	64,64,64,64	0
57	MG	1a	1797	1/1	0.83	0.11	56,56,56,56	0
57	MG	1A	3414	1/1	0.83	0.20	59,59,59,59	0
57	MG	2a	1648	1/1	0.83	0.24	69,69,69,69	0
57	MG	1A	3666	1/1	0.83	0.17	44,44,44,44	0
57	MG	1A	3777	1/1	0.83	0.24	31,31,31,31	0
57	MG	2a	1654	1/1	0.83	0.11	65,65,65,65	0
57	MG	2a	1655	1/1	0.83	0.09	73,73,73,73	0
57	MG	1a	1681	1/1	0.83	0.49	71,71,71,71	0
57	MG	1A	3942	1/1	0.83	0.15	49,49,49,49	0
57	MG	1b	301	1/1	0.83	0.47	80,80,80,80	0
57	MG	1A	3531	1/1	0.83	0.20	69,69,69,69	0
57	MG	2a	1676	1/1	0.83	0.14	64,64,64,64	0
57	MG	1A	4074	1/1	0.83	0.29	64,64,64,64	0
57	MG	2A	3653	1/1	0.83	0.15	54,54,54,54	0
57	MG	1A	3343	1/1	0.83	0.20	59,59,59,59	0
57	MG	2A	3525	1/1	0.83	0.21	84,84,84,84	0
57	MG	1A	3542	1/1	0.83	0.22	66,66,66,66	0
57	MG	1A	3547	1/1	0.83	0.28	52,52,52,52	0
57	MG	1a	1709	1/1	0.83	0.16	67,67,67,67	0
57	MG	2A	3351	1/1	0.83	0.14	54,54,54,54	0
57	MG	1A	3436	1/1	0.83	0.14	77,77,77,77	0
57	MG	1A	3437	1/1	0.83	0.14	47,47,47,47	0
57	MG	1A	3308	1/1	0.83	0.16	49,49,49,49	0
57	MG	1A	3264	1/1	0.83	0.25	44,44,44,44	0
57	MG	1a	1623	1/1	0.83	0.12	68,68,68,68	0
57	MG	2a	1754	1/1	0.83	0.29	57,57,57,57	0
57	MG	2A	3730	1/1	0.83	0.33	66,66,66,66	0
57	MG	2a	1765	1/1	0.83	0.32	68,68,68,68	0
57	MG	2a	1778	1/1	0.83	0.11	72,72,72,72	0
57	MG	1a	1736	1/1	0.83	0.27	54,54,54,54	0
57	MG	1A	3895	1/1	0.83	0.19	35,35,35,35	0
57	MG	2l	203	1/1	0.83	0.12	56,56,56,56	0
57	MG	2B	204	1/1	0.83	0.29	67,67,67,67	0
57	MG	2A	3395	1/1	0.83	0.14	63,63,63,63	0
57	MG	1B	208	1/1	0.83	0.36	59,59,59,59	0
57	MG	1a	1638	1/1	0.83	0.17	50,50,50,50	0
57	MG	20	101	1/1	0.83	0.16	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3561	1/1	0.84	0.12	73,73,73,73	0
57	MG	2A	3178	1/1	0.84	0.12	57,57,57,57	0
57	MG	1a	1804	1/1	0.84	0.10	67,67,67,67	0
57	MG	1A	3844	1/1	0.84	0.12	33,33,33,33	0
57	MG	2a	1612	1/1	0.84	0.14	59,59,59,59	0
57	MG	1A	3845	1/1	0.84	0.18	50,50,50,50	0
57	MG	2a	1617	1/1	0.84	0.19	67,67,67,67	0
57	MG	1A	3758	1/1	0.84	0.10	62,62,62,62	0
57	MG	1A	3589	1/1	0.84	0.27	58,58,58,58	0
57	MG	1S	203	1/1	0.84	0.13	63,63,63,63	0
57	MG	1a	1824	1/1	0.84	0.08	79,79,79,79	0
57	MG	1A	3428	1/1	0.84	0.14	56,56,56,56	0
57	MG	2A	3600	1/1	0.84	0.14	57,57,57,57	0
57	MG	2A	3049	1/1	0.84	0.20	63,63,63,63	0
57	MG	1A	3676	1/1	0.84	0.22	31,31,31,31	0
57	MG	2A	3437	1/1	0.84	0.17	45,45,45,45	0
57	MG	2A	3440	1/1	0.84	0.13	40,40,40,40	0
57	MG	2A	3617	1/1	0.84	0.20	43,43,43,43	0
57	MG	2A	3051	1/1	0.84	0.18	68,68,68,68	0
57	MG	1Z	3701	1/1	0.84	0.22	60,60,60,60	0
57	MG	1A	3454	1/1	0.84	0.17	62,62,62,62	0
57	MG	2A	3055	1/1	0.84	0.15	65,65,65,65	0
57	MG	2A	3253	1/1	0.84	0.24	63,63,63,63	0
57	MG	1A	3906	1/1	0.84	0.28	46,46,46,46	0
57	MG	15	108	1/1	0.84	0.27	40,40,40,40	0
57	MG	2A	3066	1/1	0.84	0.27	51,51,51,51	0
57	MG	2a	1665	1/1	0.84	0.21	67,67,67,67	0
57	MG	2A	3261	1/1	0.84	0.15	54,54,54,54	0
57	MG	1A	3787	1/1	0.84	0.09	45,45,45,45	0
57	MG	1A	3375	1/1	0.84	0.31	53,53,53,53	0
57	MG	2A	3085	1/1	0.84	0.11	62,62,62,62	0
57	MG	2A	3667	1/1	0.84	0.16	41,41,41,41	0
57	MG	2A	3088	1/1	0.84	0.10	47,47,47,47	0
57	MG	2A	3094	1/1	0.84	0.07	66,66,66,66	0
57	MG	1A	3648	1/1	0.84	0.15	40,40,40,40	0
57	MG	2A	3287	1/1	0.84	0.30	48,48,48,48	0
57	MG	2a	1707	1/1	0.84	0.09	70,70,70,70	0
57	MG	1A	3970	1/1	0.84	0.10	52,52,52,52	0
57	MG	1a	1618	1/1	0.84	0.10	48,48,48,48	0
57	MG	2A	3307	1/1	0.84	0.10	69,69,69,69	0
57	MG	1x	103	1/1	0.84	0.12	61,61,61,61	0
57	MG	2A	3114	1/1	0.84	0.13	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3319	1/1	0.84	0.18	56,56,56,56	0
57	MG	1x	105	1/1	0.84	0.13	59,59,59,59	0
57	MG	1A	3820	1/1	0.84	0.18	46,46,46,46	0
57	MG	1a	1696	1/1	0.84	0.21	72,72,72,72	0
57	MG	1a	1787	1/1	0.84	0.08	57,57,57,57	0
57	MG	2a	1779	1/1	0.84	0.16	62,62,62,62	0
57	MG	2A	3166	1/1	0.84	0.45	59,59,59,59	0
57	MG	2Q	201	1/1	0.84	0.15	53,53,53,53	0
57	MG	2X	101	1/1	0.84	0.18	51,51,51,51	0
57	MG	2Z	301	1/1	0.84	0.15	76,76,76,76	0
57	MG	2x	101	1/1	0.84	0.16	48,48,48,48	0
57	MG	2A	3366	1/1	0.84	0.28	68,68,68,68	0
57	MG	1a	1697	1/1	0.84	0.14	59,59,59,59	0
57	MG	1A	3332	1/1	0.84	0.24	42,42,42,42	0
57	MG	1a	1702	1/1	0.84	0.21	67,67,67,67	0
57	MG	1A	4013	1/1	0.85	0.15	53,53,53,53	0
57	MG	2A	3107	1/1	0.85	0.08	62,62,62,62	0
57	MG	1A	3891	1/1	0.85	0.12	46,46,46,46	0
57	MG	2A	3343	1/1	0.85	0.25	58,58,58,58	0
57	MG	2A	3349	1/1	0.85	0.16	53,53,53,53	0
57	MG	2A	3116	1/1	0.85	0.15	64,64,64,64	0
57	MG	1A	3469	1/1	0.85	0.25	56,56,56,56	0
57	MG	2A	3354	1/1	0.85	0.12	71,71,71,71	0
57	MG	2a	1610	1/1	0.85	0.07	73,73,73,73	0
57	MG	2A	3133	1/1	0.85	0.10	59,59,59,59	0
57	MG	2A	3138	1/1	0.85	0.19	53,53,53,53	0
57	MG	2A	3565	1/1	0.85	0.12	75,75,75,75	0
57	MG	2A	3567	1/1	0.85	0.09	68,68,68,68	0
57	MG	2A	3145	1/1	0.85	0.14	56,56,56,56	0
57	MG	1A	3263	1/1	0.85	0.30	58,58,58,58	0
57	MG	1A	4023	1/1	0.85	0.10	41,41,41,41	0
57	MG	1A	3416	1/1	0.85	0.10	43,43,43,43	0
57	MG	1A	3559	1/1	0.85	0.26	55,55,55,55	0
57	MG	1A	3089	1/1	0.85	0.17	50,50,50,50	0
57	MG	1U	202	1/1	0.85	0.27	40,40,40,40	0
57	MG	2A	3586	1/1	0.85	0.15	39,39,39,39	0
57	MG	2A	3589	1/1	0.85	0.26	58,58,58,58	0
57	MG	2A	3590	1/1	0.85	0.15	62,62,62,62	0
57	MG	1A	3422	1/1	0.85	0.15	49,49,49,49	0
57	MG	1A	4037	1/1	0.85	0.51	72,72,72,72	0
57	MG	1A	3344	1/1	0.85	0.38	37,37,37,37	0
57	MG	1A	3595	1/1	0.85	0.17	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	10	106	1/1	0.85	0.06	46,46,46,46	0
57	MG	1A	3355	1/1	0.85	0.22	58,58,58,58	0
57	MG	1A	3164	1/1	0.85	0.12	55,55,55,55	0
57	MG	2A	3431	1/1	0.85	0.17	48,48,48,48	0
57	MG	1A	3625	1/1	0.85	0.14	37,37,37,37	0
57	MG	2A	3435	1/1	0.85	0.20	56,56,56,56	0
57	MG	1A	3950	1/1	0.85	0.19	58,58,58,58	0
57	MG	1A	3635	1/1	0.85	0.17	58,58,58,58	0
57	MG	1A	3638	1/1	0.85	0.11	34,34,34,34	0
57	MG	2A	3216	1/1	0.85	0.19	60,60,60,60	0
57	MG	1A	3641	1/1	0.85	0.17	29,29,29,29	0
57	MG	1A	3374	1/1	0.85	0.43	43,43,43,43	0
57	MG	1A	3448	1/1	0.85	0.44	62,62,62,62	0
57	MG	1A	3238	1/1	0.85	0.19	42,42,42,42	0
57	MG	1A	4071	1/1	0.85	0.10	46,46,46,46	0
57	MG	1A	3827	1/1	0.85	0.20	61,61,61,61	0
57	MG	2A	3476	1/1	0.85	0.22	52,52,52,52	0
57	MG	2A	3689	1/1	0.85	0.15	64,64,64,64	0
57	MG	1A	3378	1/1	0.85	0.22	53,53,53,53	0
57	MG	1A	3535	1/1	0.85	0.18	69,69,69,69	0
57	MG	1A	3289	1/1	0.85	0.24	48,48,48,48	0
57	MG	1a	1808	1/1	0.85	0.07	49,49,49,49	0
57	MG	1A	3165	1/1	0.85	0.22	45,45,45,45	0
57	MG	1A	3849	1/1	0.85	0.16	37,37,37,37	0
57	MG	1A	3989	1/1	0.85	0.11	57,57,57,57	0
57	MG	1A	3696	1/1	0.85	0.25	53,53,53,53	0
57	MG	2A	3082	1/1	0.85	0.24	60,60,60,60	0
57	MG	1A	3994	1/1	0.85	0.26	73,73,73,73	0
57	MG	1A	3861	1/1	0.85	0.26	35,35,35,35	0
57	MG	2B	212	1/1	0.85	0.08	65,65,65,65	0
57	MG	1A	3341	1/1	0.85	0.14	52,52,52,52	0
57	MG	1A	3706	1/1	0.85	0.12	36,36,36,36	0
57	MG	2A	3306	1/1	0.85	0.20	62,62,62,62	0
57	MG	1a	1684	1/1	0.85	0.11	58,58,58,58	0
57	MG	1A	3880	1/1	0.85	0.30	35,35,35,35	0
57	MG	2A	3514	1/1	0.86	0.42	68,68,68,68	0
57	MG	1A	3492	1/1	0.86	0.17	36,36,36,36	0
57	MG	1A	3596	1/1	0.86	0.23	43,43,43,43	0
57	MG	1A	3690	1/1	0.86	0.10	56,56,56,56	0
57	MG	2A	3273	1/1	0.86	0.18	58,58,58,58	0
57	MG	1a	1602	1/1	0.86	0.09	62,62,62,62	0
57	MG	1A	4028	1/1	0.86	0.08	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3863	1/1	0.86	0.10	50,50,50,50	0
57	MG	1r	101	1/1	0.86	0.14	68,68,68,68	0
57	MG	1A	3962	1/1	0.86	0.21	80,80,80,80	0
57	MG	2A	3299	1/1	0.86	0.32	64,64,64,64	0
57	MG	2A	3302	1/1	0.86	0.29	64,64,64,64	0
57	MG	1v	101	1/1	0.86	0.20	71,71,71,71	0
57	MG	2A	3305	1/1	0.86	0.45	67,67,67,67	0
57	MG	1a	1616	1/1	0.86	0.11	63,63,63,63	0
57	MG	1a	1720	1/1	0.86	0.13	67,67,67,67	0
57	MG	1A	3964	1/1	0.86	0.23	43,43,43,43	0
57	MG	1a	1728	1/1	0.86	0.19	58,58,58,58	0
57	MG	2A	3128	1/1	0.86	0.22	61,61,61,61	0
57	MG	2A	3337	1/1	0.86	0.18	61,61,61,61	0
57	MG	1A	3307	1/1	0.86	0.26	63,63,63,63	0
57	MG	1a	1624	1/1	0.86	0.10	64,64,64,64	0
57	MG	1A	3765	1/1	0.86	0.07	42,42,42,42	0
57	MG	1A	3230	1/1	0.86	0.19	40,40,40,40	0
57	MG	2A	3151	1/1	0.86	0.12	45,45,45,45	0
57	MG	2A	3570	1/1	0.86	0.11	57,57,57,57	0
57	MG	1x	110	1/1	0.86	0.13	69,69,69,69	0
57	MG	1A	3775	1/1	0.86	0.18	34,34,34,34	0
57	MG	1B	236	1/1	0.86	0.18	40,40,40,40	0
57	MG	1A	3699	1/1	0.86	0.19	31,31,31,31	0
57	MG	1A	3258	1/1	0.86	0.23	38,38,38,38	0
57	MG	2A	3174	1/1	0.86	0.13	60,60,60,60	0
57	MG	1y	104	1/1	0.86	0.19	87,87,87,87	0
57	MG	1A	3471	1/1	0.86	0.13	66,66,66,66	0
57	MG	2A	3179	1/1	0.86	0.16	68,68,68,68	0
57	MG	2A	3596	1/1	0.86	0.14	68,68,68,68	0
57	MG	2A	3184	1/1	0.86	0.31	37,37,37,37	0
57	MG	1A	3792	1/1	0.86	0.21	53,53,53,53	0
57	MG	1F	312	1/1	0.86	0.19	56,56,56,56	0
57	MG	2a	1659	1/1	0.86	0.12	62,62,62,62	0
57	MG	2a	1660	1/1	0.86	0.09	56,56,56,56	0
57	MG	2A	3194	1/1	0.86	0.19	52,52,52,52	0
57	MG	2A	3197	1/1	0.86	0.18	64,64,64,64	0
57	MG	1A	3407	1/1	0.86	0.15	45,45,45,45	0
57	MG	2a	1673	1/1	0.86	0.20	57,57,57,57	0
57	MG	2A	3619	1/1	0.86	0.13	44,44,44,44	0
57	MG	2A	3202	1/1	0.86	0.17	48,48,48,48	0
57	MG	2A	3022	1/1	0.86	0.12	50,50,50,50	0
57	MG	1A	3527	1/1	0.86	0.17	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1R	201	1/1	0.86	0.34	56,56,56,56	0
57	MG	1A	3560	1/1	0.86	0.25	63,63,63,63	0
57	MG	2a	1696	1/1	0.86	0.33	66,66,66,66	0
57	MG	1a	1793	1/1	0.86	0.06	56,56,56,56	0
57	MG	1A	3348	1/1	0.86	0.21	58,58,58,58	0
57	MG	2a	1704	1/1	0.86	0.11	56,56,56,56	0
57	MG	1a	1803	1/1	0.86	0.19	68,68,68,68	0
57	MG	2a	1711	1/1	0.86	0.14	71,71,71,71	0
57	MG	1A	3410	1/1	0.86	0.20	49,49,49,49	0
57	MG	2A	3224	1/1	0.86	0.13	58,58,58,58	0
57	MG	1W	201	1/1	0.86	0.36	44,44,44,44	0
57	MG	2A	3659	1/1	0.86	0.07	77,77,77,77	0
57	MG	2A	3662	1/1	0.86	0.17	60,60,60,60	0
57	MG	2A	3230	1/1	0.86	0.13	63,63,63,63	0
57	MG	1a	1690	1/1	0.86	0.20	74,74,74,74	0
57	MG	2a	1757	1/1	0.86	0.08	59,59,59,59	0
57	MG	2a	1759	1/1	0.86	0.13	56,56,56,56	0
57	MG	2A	3680	1/1	0.86	0.07	69,69,69,69	0
57	MG	2A	3460	1/1	0.86	0.12	73,73,73,73	0
57	MG	2a	1767	1/1	0.86	0.20	57,57,57,57	0
57	MG	2a	1770	1/1	0.86	0.20	65,65,65,65	0
57	MG	1A	3842	1/1	0.86	0.12	55,55,55,55	0
57	MG	2A	3469	1/1	0.86	0.22	65,65,65,65	0
57	MG	1A	3461	1/1	0.86	0.16	38,38,38,38	0
57	MG	2A	3693	1/1	0.86	0.04	63,63,63,63	0
57	MG	2A	3058	1/1	0.86	0.20	55,55,55,55	0
57	MG	1a	1814	1/1	0.86	0.10	64,64,64,64	0
57	MG	2A	3255	1/1	0.86	0.14	55,55,55,55	0
57	MG	1A	3743	1/1	0.86	0.08	62,62,62,62	0
57	MG	1A	3752	1/1	0.86	0.23	21,21,21,21	0
57	MG	1a	1818	1/1	0.86	0.05	62,62,62,62	0
57	MG	2A	3512	1/1	0.86	0.23	42,42,42,42	0
57	MG	1A	4078	1/1	0.87	0.16	28,28,28,28	0
57	MG	2a	1601	1/1	0.87	0.14	53,53,53,53	0
57	MG	2A	3180	1/1	0.87	0.14	56,56,56,56	0
57	MG	2A	3182	1/1	0.87	0.19	55,55,55,55	0
57	MG	1A	3888	1/1	0.87	0.11	50,50,50,50	0
57	MG	2a	1609	1/1	0.87	0.12	68,68,68,68	0
57	MG	1A	4090	1/1	0.87	0.24	50,50,50,50	0
57	MG	2A	3017	1/1	0.87	0.12	56,56,56,56	0
57	MG	2A	3189	1/1	0.87	0.28	43,43,43,43	0
57	MG	2A	3193	1/1	0.87	0.08	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	4093	1/1	0.87	0.19	55,55,55,55	0
57	MG	2A	3196	1/1	0.87	0.28	52,52,52,52	0
57	MG	1A	3988	1/1	0.87	0.13	60,60,60,60	0
57	MG	1A	3319	1/1	0.87	0.15	51,51,51,51	0
57	MG	1A	3674	1/1	0.87	0.17	40,40,40,40	0
57	MG	1A	3250	1/1	0.87	0.15	56,56,56,56	0
57	MG	2a	1631	1/1	0.87	0.08	64,64,64,64	0
57	MG	2a	1633	1/1	0.87	0.19	67,67,67,67	0
57	MG	2A	3593	1/1	0.87	0.07	47,47,47,47	0
57	MG	2A	3043	1/1	0.87	0.15	51,51,51,51	0
57	MG	1A	3913	1/1	0.87	0.21	36,36,36,36	0
57	MG	2A	3417	1/1	0.87	0.16	35,35,35,35	0
57	MG	1a	1789	1/1	0.87	0.06	55,55,55,55	0
57	MG	1A	4000	1/1	0.87	0.18	28,28,28,28	0
57	MG	2A	3613	1/1	0.87	0.18	56,56,56,56	0
57	MG	1a	1643	1/1	0.87	0.14	69,69,69,69	0
57	MG	2A	3433	1/1	0.87	0.09	56,56,56,56	0
57	MG	1A	3051	1/1	0.87	0.24	42,42,42,42	0
57	MG	1a	1802	1/1	0.87	0.10	52,52,52,52	0
57	MG	1A	3689	1/1	0.87	0.28	50,50,50,50	0
57	MG	1A	3292	1/1	0.87	0.17	60,60,60,60	0
57	MG	2A	3637	1/1	0.87	0.09	67,67,67,67	0
57	MG	2A	3227	1/1	0.87	0.20	59,59,59,59	0
57	MG	1A	3781	1/1	0.87	0.18	16,16,16,16	0
57	MG	2a	1669	1/1	0.87	0.12	52,52,52,52	0
57	MG	2A	3231	1/1	0.87	0.10	65,65,65,65	0
57	MG	1a	1664	1/1	0.87	0.16	68,68,68,68	0
57	MG	1B	229	1/1	0.87	0.14	61,61,61,61	0
57	MG	1A	3500	1/1	0.87	0.50	49,49,49,49	0
57	MG	1A	3572	1/1	0.87	0.18	51,51,51,51	0
57	MG	2a	1684	1/1	0.87	0.09	76,76,76,76	0
57	MG	1A	3502	1/1	0.87	0.33	60,60,60,60	0
57	MG	1A	3207	1/1	0.87	0.22	61,61,61,61	0
57	MG	1A	3945	1/1	0.87	0.16	60,60,60,60	0
57	MG	1a	1819	1/1	0.87	0.12	56,56,56,56	0
57	MG	1E	313	1/1	0.87	0.21	31,31,31,31	0
57	MG	1A	3064	1/1	0.87	0.17	47,47,47,47	0
57	MG	1A	3107	1/1	0.87	0.53	34,34,34,34	0
57	MG	2a	1705	1/1	0.87	0.10	66,66,66,66	0
57	MG	1A	3718	1/1	0.87	0.16	36,36,36,36	0
57	MG	1I	201	1/1	0.87	0.12	64,64,64,64	0
57	MG	1A	3305	1/1	0.87	0.18	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3279	1/1	0.87	0.21	68,68,68,68	0
57	MG	1A	4035	1/1	0.87	0.13	80,80,80,80	0
57	MG	1A	3955	1/1	0.87	0.15	25,25,25,25	0
57	MG	2a	1728	1/1	0.87	0.20	64,64,64,64	0
57	MG	2a	1730	1/1	0.87	0.33	72,72,72,72	0
57	MG	2a	1739	1/1	0.87	0.32	75,75,75,75	0
57	MG	2A	3120	1/1	0.87	0.23	70,70,70,70	0
57	MG	2a	1743	1/1	0.87	0.18	68,68,68,68	0
57	MG	2a	1747	1/1	0.87	0.33	61,61,61,61	0
57	MG	1A	3245	1/1	0.87	0.34	59,59,59,59	0
57	MG	1A	3958	1/1	0.87	0.15	52,52,52,52	0
57	MG	1A	3269	1/1	0.87	0.33	53,53,53,53	0
57	MG	1A	3310	1/1	0.87	0.38	66,66,66,66	0
57	MG	1A	3366	1/1	0.87	0.19	49,49,49,49	0
57	MG	1A	3373	1/1	0.87	0.21	60,60,60,60	0
57	MG	1a	1719	1/1	0.87	0.08	60,60,60,60	0
57	MG	2a	1769	1/1	0.87	0.19	60,60,60,60	0
57	MG	1A	3965	1/1	0.87	0.11	50,50,50,50	0
57	MG	1A	3747	1/1	0.87	0.21	49,49,49,49	0
57	MG	1A	3480	1/1	0.87	0.24	74,74,74,74	0
57	MG	2A	3320	1/1	0.87	0.20	55,55,55,55	0
57	MG	2T	202	1/1	0.87	0.10	60,60,60,60	0
57	MG	1A	3969	1/1	0.87	0.11	41,41,41,41	0
57	MG	1A	3435	1/1	0.87	0.10	64,64,64,64	0
57	MG	1A	3482	1/1	0.87	0.23	53,53,53,53	0
57	MG	2A	3346	1/1	0.87	0.27	43,43,43,43	0
57	MG	1A	3878	1/1	0.87	0.17	41,41,41,41	0
57	MG	2x	104	1/1	0.87	0.21	52,52,52,52	0
57	MG	27	101	1/1	0.87	0.24	63,63,63,63	0
57	MG	1A	3670	1/1	0.87	0.18	24,24,24,24	0
57	MG	1B	233	1/1	0.88	0.16	73,73,73,73	0
57	MG	2G	201	1/1	0.88	0.10	76,76,76,76	0
57	MG	1A	3312	1/1	0.88	0.13	56,56,56,56	0
57	MG	1A	3251	1/1	0.88	0.19	50,50,50,50	0
57	MG	1A	3900	1/1	0.88	0.14	37,37,37,37	0
57	MG	1A	4007	1/1	0.88	0.11	39,39,39,39	0
57	MG	1y	103	1/1	0.88	0.37	77,77,77,77	0
57	MG	1A	3904	1/1	0.88	0.18	48,48,48,48	0
57	MG	1a	1712	1/1	0.88	0.07	79,79,79,79	0
57	MG	2A	3003	1/1	0.88	0.28	61,61,61,61	0
57	MG	1A	3320	1/1	0.88	0.21	57,57,57,57	0
57	MG	2A	3517	1/1	0.88	0.28	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3114	1/1	0.88	0.38	46,46,46,46	0
57	MG	1A	4017	1/1	0.88	0.19	23,23,23,23	0
57	MG	1A	3457	1/1	0.88	0.10	59,59,59,59	0
57	MG	1A	3558	1/1	0.88	0.11	47,47,47,47	0
57	MG	2A	3238	1/1	0.88	0.33	63,63,63,63	0
57	MG	1A	3926	1/1	0.88	0.23	41,41,41,41	0
57	MG	1Q	204	1/1	0.88	0.16	54,54,54,54	0
57	MG	1a	1729	1/1	0.88	0.35	65,65,65,65	0
57	MG	1A	4026	1/1	0.88	0.12	42,42,42,42	0
57	MG	1A	3271	1/1	0.88	0.27	42,42,42,42	0
57	MG	2A	3256	1/1	0.88	0.39	75,75,75,75	0
57	MG	2A	3258	1/1	0.88	0.09	53,53,53,53	0
57	MG	2a	1625	1/1	0.88	0.28	57,57,57,57	0
57	MG	1a	1738	1/1	0.88	0.23	62,62,62,62	0
57	MG	1A	3767	1/1	0.88	0.28	50,50,50,50	0
57	MG	1a	1744	1/1	0.88	0.15	67,67,67,67	0
57	MG	1a	1751	1/1	0.88	0.08	54,54,54,54	0
57	MG	1a	1754	1/1	0.88	0.17	43,43,43,43	0
57	MG	1A	3131	1/1	0.88	0.28	43,43,43,43	0
57	MG	1A	3561	1/1	0.88	0.15	55,55,55,55	0
57	MG	2a	1638	1/1	0.88	0.22	57,57,57,57	0
57	MG	1A	3340	1/1	0.88	0.33	51,51,51,51	0
57	MG	2A	3059	1/1	0.88	0.20	61,61,61,61	0
57	MG	2A	3062	1/1	0.88	0.10	58,58,58,58	0
57	MG	1A	3938	1/1	0.88	0.14	32,32,32,32	0
57	MG	1A	3004	1/1	0.88	0.12	26,26,26,26	0
57	MG	1a	1778	1/1	0.88	0.13	64,64,64,64	0
57	MG	10	105	1/1	0.88	0.28	63,63,63,63	0
57	MG	1A	3574	1/1	0.88	0.34	48,48,48,48	0
57	MG	2A	3079	1/1	0.88	0.38	54,54,54,54	0
57	MG	1A	4043	1/1	0.88	0.11	42,42,42,42	0
57	MG	1A	3785	1/1	0.88	0.06	36,36,36,36	0
57	MG	18	3403	1/1	0.88	0.25	46,46,46,46	0
57	MG	2A	3091	1/1	0.88	0.17	56,56,56,56	0
57	MG	2A	3092	1/1	0.88	0.22	47,47,47,47	0
57	MG	2a	1666	1/1	0.88	0.08	59,59,59,59	0
57	MG	2A	3314	1/1	0.88	0.10	52,52,52,52	0
57	MG	1A	3691	1/1	0.88	0.12	32,32,32,32	0
57	MG	1A	3579	1/1	0.88	0.20	59,59,59,59	0
57	MG	2A	3598	1/1	0.88	0.16	57,57,57,57	0
57	MG	1a	1603	1/1	0.88	0.16	64,64,64,64	0
57	MG	1A	4048	1/1	0.88	0.18	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3694	1/1	0.88	0.13	36,36,36,36	0
57	MG	1a	1612	1/1	0.88	0.14	66,66,66,66	0
57	MG	2A	3111	1/1	0.88	0.18	64,64,64,64	0
57	MG	1A	3813	1/1	0.88	0.11	53,53,53,53	0
57	MG	2a	1694	1/1	0.88	0.07	60,60,60,60	0
57	MG	1A	4054	1/1	0.88	0.14	32,32,32,32	0
57	MG	2A	3119	1/1	0.88	0.19	49,49,49,49	0
57	MG	1A	3583	1/1	0.88	0.19	44,44,44,44	0
57	MG	1A	3427	1/1	0.88	0.13	47,47,47,47	0
57	MG	2A	3365	1/1	0.88	0.24	61,61,61,61	0
57	MG	1A	3700	1/1	0.88	0.21	26,26,26,26	0
57	MG	1A	3522	1/1	0.88	0.34	34,34,34,34	0
57	MG	1A	3840	1/1	0.88	0.15	55,55,55,55	0
57	MG	1A	4069	1/1	0.88	0.14	39,39,39,39	0
57	MG	1A	3290	1/1	0.88	0.17	54,54,54,54	0
57	MG	1A	3708	1/1	0.88	0.21	34,34,34,34	0
57	MG	2A	3155	1/1	0.88	0.15	47,47,47,47	0
57	MG	1A	3470	1/1	0.88	0.16	37,37,37,37	0
57	MG	2a	1732	1/1	0.88	0.28	56,56,56,56	0
57	MG	1A	4080	1/1	0.88	0.15	52,52,52,52	0
57	MG	1a	1827	1/1	0.88	0.33	70,70,70,70	0
57	MG	1A	3429	1/1	0.88	0.21	58,58,58,58	0
57	MG	1A	3434	1/1	0.88	0.75	52,52,52,52	0
57	MG	1e	202	1/1	0.88	0.25	55,55,55,55	0
57	MG	1A	3609	1/1	0.88	0.43	56,56,56,56	0
57	MG	2A	3681	1/1	0.88	0.24	47,47,47,47	0
57	MG	2A	3177	1/1	0.88	0.21	60,60,60,60	0
57	MG	2a	1760	1/1	0.88	0.22	54,54,54,54	0
57	MG	2a	1761	1/1	0.88	0.22	59,59,59,59	0
57	MG	1a	1663	1/1	0.88	0.22	48,48,48,48	0
57	MG	1A	3613	1/1	0.88	0.16	36,36,36,36	0
57	MG	1A	3615	1/1	0.88	0.19	25,25,25,25	0
57	MG	1A	3389	1/1	0.88	0.14	43,43,43,43	0
57	MG	1A	3870	1/1	0.88	0.07	41,41,41,41	0
57	MG	1A	3735	1/1	0.88	0.19	55,55,55,55	0
57	MG	1A	3182	1/1	0.88	0.20	51,51,51,51	0
57	MG	1A	3990	1/1	0.88	0.16	59,59,59,59	0
57	MG	1A	3992	1/1	0.88	0.05	68,68,68,68	0
57	MG	2l	201	1/1	0.88	0.10	70,70,70,70	0
57	MG	2A	3729	1/1	0.88	0.22	59,59,59,59	0
57	MG	1A	3879	1/1	0.88	0.21	36,36,36,36	0
57	MG	2A	3451	1/1	0.88	0.14	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3745	1/1	0.88	0.12	48,48,48,48	0
57	MG	1x	104	1/1	0.88	0.27	68,68,68,68	0
57	MG	1A	3746	1/1	0.88	0.12	51,51,51,51	0
57	MG	2A	3462	1/1	0.88	0.07	67,67,67,67	0
57	MG	1A	3889	1/1	0.88	0.15	40,40,40,40	0
57	MG	2A	3077	1/1	0.89	0.15	66,66,66,66	0
57	MG	1A	3556	1/1	0.89	0.31	52,52,52,52	0
57	MG	1A	3327	1/1	0.89	0.27	45,45,45,45	0
57	MG	1a	1662	1/1	0.89	0.15	63,63,63,63	0
57	MG	1A	3770	1/1	0.89	0.18	46,46,46,46	0
57	MG	2A	3531	1/1	0.89	0.08	53,53,53,53	0
57	MG	1A	3002	1/1	0.89	0.16	50,50,50,50	0
57	MG	1a	1666	1/1	0.89	0.14	65,65,65,65	0
57	MG	2A	3272	1/1	0.89	0.13	61,61,61,61	0
57	MG	1A	3405	1/1	0.89	0.60	46,46,46,46	0
57	MG	1a	1673	1/1	0.89	0.10	65,65,65,65	0
57	MG	1A	3920	1/1	0.89	0.14	32,32,32,32	0
57	MG	2a	1608	1/1	0.89	0.10	68,68,68,68	0
57	MG	1A	3493	1/1	0.89	0.16	46,46,46,46	0
57	MG	1A	3451	1/1	0.89	0.33	44,44,44,44	0
57	MG	2A	3106	1/1	0.89	0.19	50,50,50,50	0
57	MG	1a	1829	1/1	0.89	0.19	60,60,60,60	0
57	MG	1A	3929	1/1	0.89	0.15	31,31,31,31	0
57	MG	1A	3452	1/1	0.89	0.37	36,36,36,36	0
57	MG	1d	301	1/1	0.89	0.20	58,58,58,58	0
57	MG	1A	3361	1/1	0.89	0.22	60,60,60,60	0
57	MG	1A	3507	1/1	0.89	0.20	38,38,38,38	0
57	MG	1A	3933	1/1	0.89	0.14	33,33,33,33	0
57	MG	1A	3799	1/1	0.89	0.12	38,38,38,38	0
57	MG	1A	3809	1/1	0.89	0.13	34,34,34,34	0
57	MG	1A	3810	1/1	0.89	0.09	36,36,36,36	0
57	MG	1G	203	1/1	0.89	0.15	68,68,68,68	0
57	MG	1A	3455	1/1	0.89	0.13	30,30,30,30	0
57	MG	1A	3362	1/1	0.89	0.21	51,51,51,51	0
57	MG	1a	1703	1/1	0.89	0.20	51,51,51,51	0
57	MG	2A	3342	1/1	0.89	0.45	60,60,60,60	0
57	MG	1a	1706	1/1	0.89	0.17	58,58,58,58	0
57	MG	1O	203	1/1	0.89	0.10	55,55,55,55	0
57	MG	1A	3514	1/1	0.89	0.15	65,65,65,65	0
57	MG	1A	3948	1/1	0.89	0.12	33,33,33,33	0
57	MG	1A	3275	1/1	0.89	0.30	39,39,39,39	0
57	MG	1A	4039	1/1	0.89	0.07	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3520	1/1	0.89	0.20	62,62,62,62	0
57	MG	1A	3133	1/1	0.89	0.31	39,39,39,39	0
57	MG	2A	3360	1/1	0.89	0.32	63,63,63,63	0
57	MG	1A	3367	1/1	0.89	0.21	45,45,45,45	0
57	MG	1A	3419	1/1	0.89	0.17	63,63,63,63	0
57	MG	1a	1725	1/1	0.89	0.08	52,52,52,52	0
57	MG	1A	3369	1/1	0.89	0.42	48,48,48,48	0
57	MG	1A	3143	1/1	0.89	0.18	55,55,55,55	0
57	MG	1A	3621	1/1	0.89	0.15	38,38,38,38	0
57	MG	1A	3730	1/1	0.89	0.08	53,53,53,53	0
57	MG	2A	3384	1/1	0.89	0.15	40,40,40,40	0
57	MG	2a	1674	1/1	0.89	0.15	65,65,65,65	0
57	MG	2A	3622	1/1	0.89	0.11	51,51,51,51	0
57	MG	2a	1679	1/1	0.89	0.11	66,66,66,66	0
57	MG	1A	3534	1/1	0.89	0.14	58,58,58,58	0
57	MG	2A	3190	1/1	0.89	0.31	40,40,40,40	0
57	MG	2a	1683	1/1	0.89	0.28	64,64,64,64	0
57	MG	2A	3397	1/1	0.89	0.11	74,74,74,74	0
57	MG	2A	3636	1/1	0.89	0.21	51,51,51,51	0
57	MG	1A	3170	1/1	0.89	0.18	45,45,45,45	0
57	MG	2A	3015	1/1	0.89	0.27	46,46,46,46	0
57	MG	2A	3195	1/1	0.89	0.17	38,38,38,38	0
57	MG	2A	3414	1/1	0.89	0.12	55,55,55,55	0
57	MG	2a	1698	1/1	0.89	0.07	62,62,62,62	0
57	MG	2a	1699	1/1	0.89	0.13	73,73,73,73	0
57	MG	2A	3649	1/1	0.89	0.12	53,53,53,53	0
57	MG	1A	3179	1/1	0.89	0.18	34,34,34,34	0
57	MG	2A	3416	1/1	0.89	0.18	50,50,50,50	0
57	MG	1A	3867	1/1	0.89	0.22	49,49,49,49	0
57	MG	1A	3246	1/1	0.89	0.39	57,57,57,57	0
57	MG	1A	3642	1/1	0.89	0.16	23,23,23,23	0
57	MG	1a	1604	1/1	0.89	0.12	54,54,54,54	0
57	MG	2A	3660	1/1	0.89	0.14	54,54,54,54	0
57	MG	1A	3543	1/1	0.89	0.25	50,50,50,50	0
57	MG	1A	3748	1/1	0.89	0.12	53,53,53,53	0
57	MG	1A	3975	1/1	0.89	0.24	50,50,50,50	0
57	MG	2A	3668	1/1	0.89	0.12	53,53,53,53	0
57	MG	2A	3673	1/1	0.89	0.10	55,55,55,55	0
57	MG	2a	1736	1/1	0.89	0.24	72,72,72,72	0
57	MG	2A	3211	1/1	0.89	0.15	51,51,51,51	0
57	MG	2a	1740	1/1	0.89	0.33	69,69,69,69	0
57	MG	1A	3652	1/1	0.89	0.15	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3682	1/1	0.89	0.12	44,44,44,44	0
57	MG	1A	3478	1/1	0.89	0.28	60,60,60,60	0
57	MG	2a	1751	1/1	0.89	0.31	59,59,59,59	0
57	MG	1A	4081	1/1	0.89	0.16	58,58,58,58	0
57	MG	2A	3218	1/1	0.89	0.18	53,53,53,53	0
57	MG	2a	1755	1/1	0.89	0.23	60,60,60,60	0
57	MG	1a	1782	1/1	0.89	0.09	52,52,52,52	0
57	MG	1A	4082	1/1	0.89	0.21	44,44,44,44	0
57	MG	2A	3225	1/1	0.89	0.13	60,60,60,60	0
57	MG	1A	3987	1/1	0.89	0.18	40,40,40,40	0
57	MG	2A	3706	1/1	0.89	0.28	56,56,56,56	0
57	MG	2a	1764	1/1	0.89	0.30	67,67,67,67	0
57	MG	1A	3661	1/1	0.89	0.14	41,41,41,41	0
57	MG	2A	3056	1/1	0.89	0.12	47,47,47,47	0
57	MG	1a	1630	1/1	0.89	0.11	59,59,59,59	0
57	MG	1A	3130	1/1	0.89	0.16	74,74,74,74	0
57	MG	2A	3237	1/1	0.89	0.14	63,63,63,63	0
57	MG	2A	3472	1/1	0.89	0.18	34,34,34,34	0
57	MG	1A	3390	1/1	0.89	0.26	45,45,45,45	0
57	MG	2a	1781	1/1	0.89	0.14	67,67,67,67	0
57	MG	2A	3477	1/1	0.89	0.21	65,65,65,65	0
57	MG	2B	205	1/1	0.89	0.18	56,56,56,56	0
57	MG	1A	3893	1/1	0.89	0.22	32,32,32,32	0
57	MG	2A	3244	1/1	0.89	0.18	65,65,65,65	0
57	MG	2B	216	1/1	0.89	0.22	75,75,75,75	0
57	MG	1A	3396	1/1	0.89	0.42	46,46,46,46	0
57	MG	1A	3896	1/1	0.89	0.18	44,44,44,44	0
57	MG	2A	3067	1/1	0.89	0.11	38,38,38,38	0
57	MG	1A	4103	1/1	0.89	0.11	48,48,48,48	0
57	MG	1A	3995	1/1	0.89	0.08	44,44,44,44	0
57	MG	1B	228	1/1	0.90	0.36	73,73,73,73	0
57	MG	2A	3071	1/1	0.90	0.17	58,58,58,58	0
57	MG	1A	3843	1/1	0.90	0.15	58,58,58,58	0
57	MG	2A	3482	1/1	0.90	0.17	63,63,63,63	0
57	MG	2A	3483	1/1	0.90	0.19	60,60,60,60	0
57	MG	1A	3325	1/1	0.90	0.27	52,52,52,52	0
57	MG	1a	1810	1/1	0.90	0.08	50,50,50,50	0
57	MG	2A	3491	1/1	0.90	0.08	70,70,70,70	0
57	MG	2A	3493	1/1	0.90	0.15	70,70,70,70	0
57	MG	1A	4027	1/1	0.90	0.41	65,65,65,65	0
57	MG	2A	3500	1/1	0.90	0.14	38,38,38,38	0
57	MG	20	102	1/1	0.90	0.17	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3479	1/1	0.90	0.16	40,40,40,40	0
57	MG	2A	3083	1/1	0.90	0.20	55,55,55,55	0
57	MG	1A	3622	1/1	0.90	0.20	53,53,53,53	0
57	MG	1A	3537	1/1	0.90	0.17	48,48,48,48	0
57	MG	1A	3055	1/1	0.90	0.22	50,50,50,50	0
57	MG	2A	3520	1/1	0.90	0.21	44,44,44,44	0
57	MG	1A	3026	1/1	0.90	0.27	63,63,63,63	0
57	MG	1A	3121	1/1	0.90	0.25	38,38,38,38	0
57	MG	1a	1823	1/1	0.90	0.10	61,61,61,61	0
57	MG	1A	3544	1/1	0.90	0.28	45,45,45,45	0
57	MG	2A	3275	1/1	0.90	0.15	65,65,65,65	0
57	MG	1F	309	1/1	0.90	0.26	40,40,40,40	0
57	MG	1A	3749	1/1	0.90	0.15	50,50,50,50	0
57	MG	1A	3960	1/1	0.90	0.18	42,42,42,42	0
57	MG	2A	3539	1/1	0.90	0.12	66,66,66,66	0
57	MG	2a	1619	1/1	0.90	0.22	64,64,64,64	0
57	MG	1A	3247	1/1	0.90	0.36	62,62,62,62	0
57	MG	1A	3874	1/1	0.90	0.23	58,58,58,58	0
57	MG	2A	3288	1/1	0.90	0.31	60,60,60,60	0
57	MG	2a	1623	1/1	0.90	0.16	68,68,68,68	0
57	MG	2A	3113	1/1	0.90	0.12	42,42,42,42	0
57	MG	2A	3545	1/1	0.90	0.18	46,46,46,46	0
57	MG	1A	3963	1/1	0.90	0.11	54,54,54,54	0
57	MG	1A	3010	1/1	0.90	0.16	39,39,39,39	0
57	MG	1A	3549	1/1	0.90	0.26	65,65,65,65	0
57	MG	1l	202	1/1	0.90	0.09	64,64,64,64	0
57	MG	1A	3094	1/1	0.90	0.28	34,34,34,34	0
57	MG	1S	202	1/1	0.90	0.19	46,46,46,46	0
57	MG	2A	3132	1/1	0.90	0.18	53,53,53,53	0
57	MG	1A	3398	1/1	0.90	0.16	67,67,67,67	0
57	MG	2a	1641	1/1	0.90	0.17	63,63,63,63	0
57	MG	1A	3881	1/1	0.90	0.14	29,29,29,29	0
57	MG	2A	3316	1/1	0.90	0.27	53,53,53,53	0
57	MG	2A	3318	1/1	0.90	0.18	48,48,48,48	0
57	MG	1A	3886	1/1	0.90	0.26	50,50,50,50	0
57	MG	2A	3147	1/1	0.90	0.10	54,54,54,54	0
57	MG	2A	3321	1/1	0.90	0.12	55,55,55,55	0
57	MG	2A	3324	1/1	0.90	0.28	61,61,61,61	0
57	MG	2a	1656	1/1	0.90	0.15	84,84,84,84	0
57	MG	2A	3329	1/1	0.90	0.24	58,58,58,58	0
57	MG	1A	3216	1/1	0.90	0.50	40,40,40,40	0
57	MG	1Y	202	1/1	0.90	0.28	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3557	1/1	0.90	0.26	55,55,55,55	0
57	MG	2A	3157	1/1	0.90	0.09	53,53,53,53	0
57	MG	1A	3219	1/1	0.90	0.18	33,33,33,33	0
57	MG	1A	3301	1/1	0.90	0.45	68,68,68,68	0
57	MG	2A	3591	1/1	0.90	0.10	61,61,61,61	0
57	MG	2a	1670	1/1	0.90	0.08	63,63,63,63	0
57	MG	2a	1671	1/1	0.90	0.19	55,55,55,55	0
57	MG	2A	3164	1/1	0.90	0.21	61,61,61,61	0
57	MG	1Z	3703	1/1	0.90	0.25	52,52,52,52	0
57	MG	1a	1718	1/1	0.90	0.13	70,70,70,70	0
57	MG	1A	4067	1/1	0.90	0.12	34,34,34,34	0
57	MG	1A	3505	1/1	0.90	0.23	34,34,34,34	0
57	MG	1x	111	1/1	0.90	0.09	62,62,62,62	0
57	MG	10	107	1/1	0.90	0.13	59,59,59,59	0
57	MG	2A	3608	1/1	0.90	0.08	53,53,53,53	0
57	MG	1A	4070	1/1	0.90	0.12	48,48,48,48	0
57	MG	1A	3345	1/1	0.90	0.23	51,51,51,51	0
57	MG	2a	1688	1/1	0.90	0.09	62,62,62,62	0
57	MG	17	103	1/1	0.90	0.13	48,48,48,48	0
57	MG	1A	3259	1/1	0.90	0.22	48,48,48,48	0
57	MG	1A	3779	1/1	0.90	0.26	26,26,26,26	0
57	MG	2A	3624	1/1	0.90	0.15	76,76,76,76	0
57	MG	2A	3625	1/1	0.90	0.17	65,65,65,65	0
57	MG	2A	3627	1/1	0.90	0.14	72,72,72,72	0
57	MG	2A	3373	1/1	0.90	0.18	62,62,62,62	0
57	MG	18	3406	1/1	0.90	0.37	53,53,53,53	0
57	MG	1A	3224	1/1	0.90	0.22	39,39,39,39	0
57	MG	2A	3386	1/1	0.90	0.18	72,72,72,72	0
57	MG	1A	3573	1/1	0.90	0.14	43,43,43,43	0
57	MG	2a	1709	1/1	0.90	0.11	78,78,78,78	0
57	MG	2a	1710	1/1	0.90	0.16	59,59,59,59	0
57	MG	1a	1746	1/1	0.90	0.22	57,57,57,57	0
57	MG	2A	3192	1/1	0.90	0.14	54,54,54,54	0
57	MG	2A	3643	1/1	0.90	0.08	66,66,66,66	0
57	MG	2A	3399	1/1	0.90	0.11	35,35,35,35	0
57	MG	1A	3358	1/1	0.90	0.33	82,82,82,82	0
57	MG	1A	4086	1/1	0.90	0.31	49,49,49,49	0
57	MG	2A	3408	1/1	0.90	0.16	48,48,48,48	0
57	MG	1a	1757	1/1	0.90	0.26	73,73,73,73	0
57	MG	2A	3410	1/1	0.90	0.14	63,63,63,63	0
57	MG	2a	1737	1/1	0.90	0.16	64,64,64,64	0
57	MG	1A	3518	1/1	0.90	0.14	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3026	1/1	0.90	0.23	54,54,54,54	0
57	MG	1A	3463	1/1	0.90	0.18	45,45,45,45	0
57	MG	2A	3037	1/1	0.90	0.27	57,57,57,57	0
57	MG	1A	3097	1/1	0.90	0.19	37,37,37,37	0
57	MG	2A	3424	1/1	0.90	0.17	33,33,33,33	0
57	MG	1A	4094	1/1	0.90	0.14	41,41,41,41	0
57	MG	2A	3429	1/1	0.90	0.09	48,48,48,48	0
57	MG	2A	3677	1/1	0.90	0.07	56,56,56,56	0
57	MG	2A	3679	1/1	0.90	0.11	45,45,45,45	0
57	MG	2A	3042	1/1	0.90	0.16	54,54,54,54	0
57	MG	1A	3102	1/1	0.90	0.29	42,42,42,42	0
57	MG	1a	1777	1/1	0.90	0.08	71,71,71,71	0
57	MG	1A	4096	1/1	0.90	0.28	54,54,54,54	0
57	MG	1A	3593	1/1	0.90	0.19	34,34,34,34	0
57	MG	1a	1627	1/1	0.90	0.10	59,59,59,59	0
57	MG	1A	3233	1/1	0.90	0.12	36,36,36,36	0
57	MG	2a	1768	1/1	0.90	0.12	61,61,61,61	0
57	MG	1A	3147	1/1	0.90	0.16	34,34,34,34	0
57	MG	1A	3274	1/1	0.90	0.22	52,52,52,52	0
57	MG	2A	3697	1/1	0.90	0.11	47,47,47,47	0
57	MG	1A	3601	1/1	0.90	0.42	36,36,36,36	0
57	MG	1A	3530	1/1	0.90	0.23	55,55,55,55	0
57	MG	2A	3707	1/1	0.90	0.22	72,72,72,72	0
57	MG	2A	3708	1/1	0.90	0.11	56,56,56,56	0
57	MG	2a	1785	1/1	0.90	0.11	69,69,69,69	0
57	MG	1A	3936	1/1	0.90	0.23	55,55,55,55	0
57	MG	1A	3937	1/1	0.90	0.10	52,52,52,52	0
57	MG	2q	202	1/1	0.90	0.13	75,75,75,75	0
57	MG	2A	3061	1/1	0.90	0.13	39,39,39,39	0
57	MG	2A	3461	1/1	0.90	0.09	65,65,65,65	0
57	MG	1a	1645	1/1	0.90	0.13	65,65,65,65	0
57	MG	2A	3236	1/1	0.90	0.15	63,63,63,63	0
57	MG	1a	1647	1/1	0.90	0.12	52,52,52,52	0
57	MG	1A	3322	1/1	0.90	0.15	29,29,29,29	0
57	MG	1A	3533	1/1	0.90	0.12	81,81,81,81	0
57	MG	1A	3771	1/1	0.91	0.22	44,44,44,44	0
57	MG	2A	3720	1/1	0.91	0.10	41,41,41,41	0
57	MG	1A	3152	1/1	0.91	0.23	40,40,40,40	0
57	MG	1A	3158	1/1	0.91	0.11	49,49,49,49	0
57	MG	1A	3620	1/1	0.91	0.16	39,39,39,39	0
57	MG	2A	3450	1/1	0.91	0.11	44,44,44,44	0
57	MG	1a	1665	1/1	0.91	0.12	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3199	1/1	0.91	0.16	64,64,64,64	0
57	MG	2A	3201	1/1	0.91	0.18	77,77,77,77	0
57	MG	1A	3511	1/1	0.91	0.11	64,64,64,64	0
57	MG	2B	211	1/1	0.91	0.29	62,62,62,62	0
57	MG	1A	3956	1/1	0.91	0.24	26,26,26,26	0
57	MG	2B	213	1/1	0.91	0.23	64,64,64,64	0
57	MG	2B	214	1/1	0.91	0.23	70,70,70,70	0
57	MG	1a	1672	1/1	0.91	0.21	67,67,67,67	0
57	MG	1A	3425	1/1	0.91	0.11	40,40,40,40	0
57	MG	2B	218	1/1	0.91	0.22	64,64,64,64	0
57	MG	2E	303	1/1	0.91	0.15	43,43,43,43	0
57	MG	1A	3006	1/1	0.91	0.21	54,54,54,54	0
57	MG	1A	3786	1/1	0.91	0.15	61,61,61,61	0
57	MG	1A	3634	1/1	0.91	0.14	52,52,52,52	0
57	MG	1A	3284	1/1	0.91	0.12	42,42,42,42	0
57	MG	2W	201	1/1	0.91	0.27	40,40,40,40	0
57	MG	1A	3794	1/1	0.91	0.17	64,64,64,64	0
57	MG	1A	3072	1/1	0.91	0.30	52,52,52,52	0
57	MG	1A	3433	1/1	0.91	0.16	41,41,41,41	0
57	MG	1B	206	1/1	0.91	0.27	47,47,47,47	0
57	MG	2A	3008	1/1	0.91	0.21	56,56,56,56	0
57	MG	2A	3485	1/1	0.91	0.14	32,32,32,32	0
57	MG	2A	3010	1/1	0.91	0.22	62,62,62,62	0
57	MG	1A	3086	1/1	0.91	0.15	35,35,35,35	0
57	MG	1A	3234	1/1	0.91	0.43	42,42,42,42	0
57	MG	2A	3495	1/1	0.91	0.16	38,38,38,38	0
57	MG	1A	3649	1/1	0.91	0.21	50,50,50,50	0
57	MG	1A	3115	1/1	0.91	0.22	42,42,42,42	0
57	MG	2A	3235	1/1	0.91	0.23	60,60,60,60	0
57	MG	2a	1606	1/1	0.91	0.12	71,71,71,71	0
57	MG	1B	226	1/1	0.91	0.16	37,37,37,37	0
57	MG	2A	3513	1/1	0.91	0.17	45,45,45,45	0
57	MG	1A	3653	1/1	0.91	0.12	72,72,72,72	0
57	MG	1A	3825	1/1	0.91	0.20	56,56,56,56	0
57	MG	2A	3241	1/1	0.91	0.17	49,49,49,49	0
57	MG	2A	3038	1/1	0.91	0.21	52,52,52,52	0
57	MG	1A	3116	1/1	0.91	0.19	30,30,30,30	0
57	MG	2A	3246	1/1	0.91	0.15	66,66,66,66	0
57	MG	2A	3247	1/1	0.91	0.10	53,53,53,53	0
57	MG	2A	3529	1/1	0.91	0.25	73,73,73,73	0
57	MG	2A	3248	1/1	0.91	0.49	57,57,57,57	0
57	MG	1A	3172	1/1	0.91	0.13	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3664	1/1	0.91	0.12	50,50,50,50	0
57	MG	1A	3981	1/1	0.91	0.11	44,44,44,44	0
57	MG	1A	3532	1/1	0.91	0.11	71,71,71,71	0
57	MG	1A	3439	1/1	0.91	0.13	54,54,54,54	0
57	MG	1A	3444	1/1	0.91	0.25	65,65,65,65	0
57	MG	1A	3118	1/1	0.91	0.14	49,49,49,49	0
57	MG	1A	3846	1/1	0.91	0.23	60,60,60,60	0
57	MG	1A	3364	1/1	0.91	0.16	43,43,43,43	0
57	MG	1A	3018	1/1	0.91	0.17	36,36,36,36	0
57	MG	1A	3687	1/1	0.91	0.17	27,27,27,27	0
57	MG	1A	3856	1/1	0.91	0.11	55,55,55,55	0
57	MG	1N	205	1/1	0.91	0.12	54,54,54,54	0
57	MG	2A	3554	1/1	0.91	0.17	60,60,60,60	0
57	MG	1A	3539	1/1	0.91	0.17	38,38,38,38	0
57	MG	1A	3128	1/1	0.91	0.20	45,45,45,45	0
57	MG	2A	3557	1/1	0.91	0.06	51,51,51,51	0
57	MG	1A	3187	1/1	0.91	0.09	44,44,44,44	0
57	MG	1P	205	1/1	0.91	0.40	49,49,49,49	0
57	MG	2A	3280	1/1	0.91	0.08	58,58,58,58	0
57	MG	1Q	203	1/1	0.91	0.18	55,55,55,55	0
57	MG	1A	3368	1/1	0.91	0.11	57,57,57,57	0
57	MG	1A	4004	1/1	0.91	0.13	54,54,54,54	0
57	MG	2a	1661	1/1	0.91	0.17	71,71,71,71	0
57	MG	2A	3068	1/1	0.91	0.18	29,29,29,29	0
57	MG	2A	3069	1/1	0.91	0.14	67,67,67,67	0
57	MG	2A	3571	1/1	0.91	0.09	66,66,66,66	0
57	MG	2a	1667	1/1	0.91	0.13	52,52,52,52	0
57	MG	1a	1753	1/1	0.91	0.11	34,34,34,34	0
57	MG	1A	3005	1/1	0.91	0.17	37,37,37,37	0
57	MG	1A	3872	1/1	0.91	0.19	42,42,42,42	0
57	MG	2A	3076	1/1	0.91	0.17	53,53,53,53	0
57	MG	1A	4012	1/1	0.91	0.12	36,36,36,36	0
57	MG	1A	3371	1/1	0.91	0.17	50,50,50,50	0
57	MG	1a	1762	1/1	0.91	0.11	41,41,41,41	0
57	MG	2A	3588	1/1	0.91	0.25	71,71,71,71	0
57	MG	1V	202	1/1	0.91	0.25	38,38,38,38	0
57	MG	1A	3257	1/1	0.91	0.19	27,27,27,27	0
57	MG	2A	3087	1/1	0.91	0.12	70,70,70,70	0
57	MG	2A	3592	1/1	0.91	0.08	52,52,52,52	0
57	MG	1A	3550	1/1	0.91	0.32	47,47,47,47	0
57	MG	1a	1776	1/1	0.91	0.18	70,70,70,70	0
57	MG	2a	1689	1/1	0.91	0.19	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3701	1/1	0.91	0.20	23,23,23,23	0
57	MG	1A	3313	1/1	0.91	0.29	52,52,52,52	0
57	MG	1A	3554	1/1	0.91	0.30	58,58,58,58	0
57	MG	1A	3882	1/1	0.91	0.16	34,34,34,34	0
57	MG	10	103	1/1	0.91	0.12	47,47,47,47	0
57	MG	2A	3338	1/1	0.91	0.51	54,54,54,54	0
57	MG	2A	3340	1/1	0.91	0.31	52,52,52,52	0
57	MG	1A	3707	1/1	0.91	0.18	33,33,33,33	0
57	MG	1A	3316	1/1	0.91	0.27	59,59,59,59	0
57	MG	1A	3058	1/1	0.91	0.30	54,54,54,54	0
57	MG	13	102	1/1	0.91	0.14	47,47,47,47	0
57	MG	1A	3384	1/1	0.91	0.21	37,37,37,37	0
57	MG	1A	3388	1/1	0.91	0.24	64,64,64,64	0
57	MG	1A	3060	1/1	0.91	0.20	49,49,49,49	0
57	MG	1A	3321	1/1	0.91	0.20	35,35,35,35	0
57	MG	1A	3899	1/1	0.91	0.21	25,25,25,25	0
57	MG	2A	3633	1/1	0.91	0.09	34,34,34,34	0
57	MG	1A	3395	1/1	0.91	0.14	48,48,48,48	0
57	MG	2A	3126	1/1	0.91	0.18	67,67,67,67	0
57	MG	1A	3903	1/1	0.91	0.15	23,23,23,23	0
57	MG	1A	3034	1/1	0.91	0.12	47,47,47,47	0
57	MG	1A	3209	1/1	0.91	0.18	34,34,34,34	0
57	MG	1A	3733	1/1	0.91	0.13	53,53,53,53	0
57	MG	2A	3645	1/1	0.91	0.06	47,47,47,47	0
57	MG	1a	1607	1/1	0.91	0.27	62,62,62,62	0
57	MG	1A	3915	1/1	0.91	0.13	46,46,46,46	0
57	MG	1A	3734	1/1	0.91	0.15	51,51,51,51	0
57	MG	1A	3326	1/1	0.91	0.23	51,51,51,51	0
57	MG	2A	3152	1/1	0.91	0.12	55,55,55,55	0
57	MG	1A	3049	1/1	0.91	0.29	32,32,32,32	0
57	MG	1a	1617	1/1	0.91	0.10	46,46,46,46	0
57	MG	1A	3483	1/1	0.91	0.27	41,41,41,41	0
57	MG	1A	4053	1/1	0.91	0.18	28,28,28,28	0
57	MG	1A	3487	1/1	0.91	0.21	39,39,39,39	0
57	MG	1a	1625	1/1	0.91	0.26	54,54,54,54	0
57	MG	2A	3666	1/1	0.91	0.13	54,54,54,54	0
57	MG	1A	3402	1/1	0.91	0.30	40,40,40,40	0
57	MG	1A	3149	1/1	0.91	0.44	30,30,30,30	0
57	MG	1A	3331	1/1	0.91	0.20	54,54,54,54	0
57	MG	1a	1633	1/1	0.91	0.24	56,56,56,56	0
57	MG	2A	3176	1/1	0.91	0.36	42,42,42,42	0
57	MG	1a	1634	1/1	0.91	0.16	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3218	1/1	0.91	0.39	39,39,39,39	0
57	MG	2a	1776	1/1	0.91	0.13	63,63,63,63	0
57	MG	1A	3333	1/1	0.91	0.12	55,55,55,55	0
57	MG	2A	3420	1/1	0.91	0.14	47,47,47,47	0
57	MG	1A	3411	1/1	0.91	0.24	51,51,51,51	0
57	MG	1A	3599	1/1	0.91	0.15	39,39,39,39	0
57	MG	2A	3690	1/1	0.91	0.10	51,51,51,51	0
57	MG	1A	3334	1/1	0.91	0.11	51,51,51,51	0
57	MG	2d	301	1/1	0.91	0.25	56,56,56,56	0
57	MG	2A	3428	1/1	0.91	0.21	41,41,41,41	0
57	MG	2A	3185	1/1	0.91	0.13	72,72,72,72	0
57	MG	1A	3336	1/1	0.91	0.25	43,43,43,43	0
57	MG	1A	3941	1/1	0.91	0.06	60,60,60,60	0
57	MG	1A	3273	1/1	0.91	0.22	36,36,36,36	0
57	MG	1A	3610	1/1	0.91	0.11	57,57,57,57	0
57	MG	1a	1653	1/1	0.91	0.16	43,43,43,43	0
57	MG	2A	3710	1/1	0.91	0.18	60,60,60,60	0
57	MG	1A	3611	1/1	0.91	0.31	48,48,48,48	0
57	MG	2A	3715	1/1	0.91	0.11	68,68,68,68	0
59	ZN	2n	501	1/1	0.91	0.07	95,95,95,95	0
61	K	2A	3330	1/1	0.91	0.23	75,75,75,75	0
57	MG	2A	3292	1/1	0.92	0.33	49,49,49,49	0
57	MG	2R	201	1/1	0.92	0.15	54,54,54,54	0
57	MG	1A	3423	1/1	0.92	0.13	56,56,56,56	0
57	MG	2A	3295	1/1	0.92	0.17	36,36,36,36	0
57	MG	2A	3125	1/1	0.92	0.22	50,50,50,50	0
57	MG	2A	3300	1/1	0.92	0.34	64,64,64,64	0
57	MG	2A	3536	1/1	0.92	0.10	33,33,33,33	0
57	MG	1A	3506	1/1	0.92	0.13	41,41,41,41	0
57	MG	20	103	1/1	0.92	0.15	64,64,64,64	0
57	MG	23	102	1/1	0.92	0.13	59,59,59,59	0
57	MG	2A	3127	1/1	0.92	0.24	66,66,66,66	0
57	MG	13	104	1/1	0.92	0.21	51,51,51,51	0
57	MG	1w	102	1/1	0.92	0.09	53,53,53,53	0
57	MG	1a	1710	1/1	0.92	0.17	63,63,63,63	0
57	MG	2A	3308	1/1	0.92	0.09	52,52,52,52	0
57	MG	1A	3919	1/1	0.92	0.10	64,64,64,64	0
57	MG	2A	3143	1/1	0.92	0.14	53,53,53,53	0
57	MG	1A	3714	1/1	0.92	0.14	42,42,42,42	0
57	MG	1A	3552	1/1	0.92	0.39	51,51,51,51	0
57	MG	1A	3349	1/1	0.92	0.33	49,49,49,49	0
57	MG	2A	3150	1/1	0.92	0.23	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3148	1/1	0.92	0.48	38,38,38,38	0
57	MG	1A	3720	1/1	0.92	0.14	54,54,54,54	0
57	MG	2a	1611	1/1	0.92	0.11	66,66,66,66	0
57	MG	2A	3154	1/1	0.92	0.13	41,41,41,41	0
57	MG	2a	1614	1/1	0.92	0.07	56,56,56,56	0
57	MG	1x	106	1/1	0.92	0.14	69,69,69,69	0
57	MG	1A	3019	1/1	0.92	0.21	43,43,43,43	0
57	MG	2a	1618	1/1	0.92	0.15	73,73,73,73	0
57	MG	1B	202	1/1	0.92	0.35	61,61,61,61	0
57	MG	1a	1723	1/1	0.92	0.13	38,38,38,38	0
57	MG	1x	112	1/1	0.92	0.20	62,62,62,62	0
57	MG	1A	3210	1/1	0.92	0.11	38,38,38,38	0
57	MG	2A	3167	1/1	0.92	0.08	57,57,57,57	0
57	MG	1A	3176	1/1	0.92	0.19	35,35,35,35	0
57	MG	2A	3572	1/1	0.92	0.10	69,69,69,69	0
57	MG	1A	3639	1/1	0.92	0.11	27,27,27,27	0
57	MG	2A	3172	1/1	0.92	0.16	51,51,51,51	0
57	MG	1a	1731	1/1	0.92	0.15	47,47,47,47	0
57	MG	1A	3214	1/1	0.92	0.14	47,47,47,47	0
57	MG	1a	1735	1/1	0.92	0.20	48,48,48,48	0
57	MG	1A	3078	1/1	0.92	0.22	48,48,48,48	0
57	MG	2A	3358	1/1	0.92	0.21	59,59,59,59	0
57	MG	2A	3359	1/1	0.92	0.09	63,63,63,63	0
57	MG	1A	3024	1/1	0.92	0.24	45,45,45,45	0
57	MG	2A	3362	1/1	0.92	0.16	38,38,38,38	0
57	MG	2A	3363	1/1	0.92	0.18	57,57,57,57	0
57	MG	1a	1739	1/1	0.92	0.12	73,73,73,73	0
57	MG	1A	4020	1/1	0.92	0.17	21,21,21,21	0
57	MG	2A	3595	1/1	0.92	0.16	40,40,40,40	0
57	MG	1a	1743	1/1	0.92	0.31	59,59,59,59	0
57	MG	1A	3335	1/1	0.92	0.25	54,54,54,54	0
57	MG	1a	1745	1/1	0.92	0.25	68,68,68,68	0
57	MG	1a	1622	1/1	0.92	0.32	63,63,63,63	0
57	MG	2A	3602	1/1	0.92	0.10	58,58,58,58	0
57	MG	2A	3018	1/1	0.92	0.22	41,41,41,41	0
57	MG	2A	3374	1/1	0.92	0.31	40,40,40,40	0
57	MG	1a	1747	1/1	0.92	0.20	57,57,57,57	0
57	MG	1A	3736	1/1	0.92	0.20	60,60,60,60	0
57	MG	2A	3023	1/1	0.92	0.38	41,41,41,41	0
57	MG	1A	3650	1/1	0.92	0.17	26,26,26,26	0
57	MG	2A	3027	1/1	0.92	0.09	46,46,46,46	0
57	MG	2a	1668	1/1	0.92	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
57	MG	2A	3621	1/1	0.92	0.27	48,48,48,48	0
57	MG	1A	3852	1/1	0.92	0.07	71,71,71,71	0
57	MG	1A	3045	1/1	0.92	0.17	35,35,35,35	0
57	MG	2A	3400	1/1	0.92	0.12	42,42,42,42	0
57	MG	1A	3855	1/1	0.92	0.10	56,56,56,56	0
57	MG	1A	3315	1/1	0.92	0.24	54,54,54,54	0
57	MG	2A	3630	1/1	0.92	0.20	61,61,61,61	0
57	MG	1A	3857	1/1	0.92	0.09	51,51,51,51	0
57	MG	1A	3441	1/1	0.92	0.15	48,48,48,48	0
57	MG	1E	306	1/1	0.92	0.10	29,29,29,29	0
57	MG	1A	3657	1/1	0.92	0.12	27,27,27,27	0
57	MG	1A	3864	1/1	0.92	0.14	21,21,21,21	0
57	MG	1A	3658	1/1	0.92	0.15	31,31,31,31	0
57	MG	1A	3252	1/1	0.92	0.17	53,53,53,53	0
57	MG	2A	3642	1/1	0.92	0.08	50,50,50,50	0
57	MG	2a	1690	1/1	0.92	0.20	61,61,61,61	0
57	MG	1A	3663	1/1	0.92	0.13	42,42,42,42	0
57	MG	1a	1780	1/1	0.92	0.12	60,60,60,60	0
57	MG	1A	3445	1/1	0.92	0.24	57,57,57,57	0
57	MG	1a	1649	1/1	0.92	0.16	45,45,45,45	0
57	MG	2A	3217	1/1	0.92	0.12	58,58,58,58	0
57	MG	1G	204	1/1	0.92	0.18	68,68,68,68	0
57	MG	2A	3220	1/1	0.92	0.19	45,45,45,45	0
57	MG	1A	3757	1/1	0.92	0.12	51,51,51,51	0
57	MG	1A	3484	1/1	0.92	0.29	43,43,43,43	0
57	MG	1a	1655	1/1	0.92	0.10	54,54,54,54	0
57	MG	1a	1657	1/1	0.92	0.18	52,52,52,52	0
57	MG	2A	3438	1/1	0.92	0.13	31,31,31,31	0
57	MG	1A	3760	1/1	0.92	0.18	36,36,36,36	0
57	MG	1a	1792	1/1	0.92	0.20	64,64,64,64	0
57	MG	1A	3588	1/1	0.92	0.27	40,40,40,40	0
57	MG	2a	1715	1/1	0.92	0.43	69,69,69,69	0
57	MG	1A	3486	1/1	0.92	0.32	41,41,41,41	0
57	MG	2a	1719	1/1	0.92	0.16	67,67,67,67	0
57	MG	2a	1720	1/1	0.92	0.14	65,65,65,65	0
57	MG	1a	1801	1/1	0.92	0.10	51,51,51,51	0
57	MG	2a	1723	1/1	0.92	0.10	61,61,61,61	0
57	MG	2a	1724	1/1	0.92	0.27	65,65,65,65	0
57	MG	1A	3590	1/1	0.92	0.16	29,29,29,29	0
57	MG	1A	3447	1/1	0.92	0.21	38,38,38,38	0
57	MG	2a	1729	1/1	0.92	0.27	63,63,63,63	0
57	MG	2A	3073	1/1	0.92	0.07	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2a	1731	1/1	0.92	0.31	61,61,61,61	0
57	MG	2A	3454	1/1	0.92	0.17	59,59,59,59	0
57	MG	2a	1733	1/1	0.92	0.28	57,57,57,57	0
57	MG	1A	3318	1/1	0.92	0.17	50,50,50,50	0
57	MG	1Q	206	1/1	0.92	0.23	34,34,34,34	0
57	MG	1a	1667	1/1	0.92	0.50	56,56,56,56	0
57	MG	1A	4057	1/1	0.92	0.19	31,31,31,31	0
57	MG	1a	1670	1/1	0.92	0.10	66,66,66,66	0
57	MG	1A	3412	1/1	0.92	0.19	51,51,51,51	0
57	MG	1A	3221	1/1	0.92	0.11	45,45,45,45	0
57	MG	2A	3695	1/1	0.92	0.21	62,62,62,62	0
57	MG	2A	3252	1/1	0.92	0.09	71,71,71,71	0
57	MG	1a	1815	1/1	0.92	0.07	64,64,64,64	0
57	MG	2A	3698	1/1	0.92	0.11	41,41,41,41	0
57	MG	2A	3701	1/1	0.92	0.23	61,61,61,61	0
57	MG	2a	1758	1/1	0.92	0.24	57,57,57,57	0
57	MG	1A	3122	1/1	0.92	0.24	45,45,45,45	0
57	MG	1A	3540	1/1	0.92	0.22	34,34,34,34	0
57	MG	1a	1677	1/1	0.92	0.17	64,64,64,64	0
57	MG	2A	3257	1/1	0.92	0.14	57,57,57,57	0
57	MG	1A	3495	1/1	0.92	0.20	41,41,41,41	0
57	MG	1A	3144	1/1	0.92	0.22	46,46,46,46	0
57	MG	2a	1766	1/1	0.92	0.29	62,62,62,62	0
57	MG	1W	206	1/1	0.92	0.15	34,34,34,34	0
57	MG	2A	3098	1/1	0.92	0.10	46,46,46,46	0
57	MG	1A	3982	1/1	0.92	0.21	57,57,57,57	0
57	MG	1A	3985	1/1	0.92	0.06	62,62,62,62	0
57	MG	2a	1775	1/1	0.92	0.23	76,76,76,76	0
57	MG	2A	3723	1/1	0.92	0.10	69,69,69,69	0
57	MG	2A	3268	1/1	0.92	0.24	54,54,54,54	0
57	MG	2A	3498	1/1	0.92	0.13	45,45,45,45	0
57	MG	1A	3167	1/1	0.92	0.23	39,39,39,39	0
57	MG	2A	3503	1/1	0.92	0.14	50,50,50,50	0
57	MG	2a	1782	1/1	0.92	0.20	62,62,62,62	0
57	MG	2A	3504	1/1	0.92	0.18	59,59,59,59	0
57	MG	1A	3546	1/1	0.92	0.34	41,41,41,41	0
57	MG	2A	3508	1/1	0.92	0.12	41,41,41,41	0
57	MG	2f	201	1/1	0.92	0.16	52,52,52,52	0
57	MG	1A	3901	1/1	0.92	0.14	29,29,29,29	0
57	MG	2A	3108	1/1	0.92	0.14	43,43,43,43	0
57	MG	2A	3110	1/1	0.92	0.09	55,55,55,55	0
57	MG	2q	203	1/1	0.92	0.09	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3516	1/1	0.92	0.11	50,50,50,50	0
57	MG	1a	1694	1/1	0.92	0.19	59,59,59,59	0
57	MG	1A	3501	1/1	0.92	0.12	46,46,46,46	0
57	MG	1A	3612	1/1	0.92	0.19	24,24,24,24	0
57	MG	2D	304	1/1	0.92	0.15	62,62,62,62	0
57	MG	1A	3126	1/1	0.92	0.27	36,36,36,36	0
57	MG	1A	3614	1/1	0.92	0.13	54,54,54,54	0
57	MG	2F	302	1/1	0.92	0.12	50,50,50,50	0
57	MG	1l	103	1/1	0.92	0.17	39,39,39,39	0
57	MG	1a	1606	1/1	0.93	0.19	53,53,53,53	0
57	MG	1a	1756	1/1	0.93	0.14	56,56,56,56	0
57	MG	1A	3276	1/1	0.93	0.12	40,40,40,40	0
57	MG	1A	3902	1/1	0.93	0.20	27,27,27,27	0
57	MG	2E	305	1/1	0.93	0.17	39,39,39,39	0
57	MG	1a	1759	1/1	0.93	0.13	58,58,58,58	0
57	MG	2A	3063	1/1	0.93	0.22	52,52,52,52	0
57	MG	2F	306	1/1	0.93	0.23	62,62,62,62	0
57	MG	1A	3181	1/1	0.93	0.17	47,47,47,47	0
57	MG	2O	201	1/1	0.93	0.16	70,70,70,70	0
57	MG	1A	3059	1/1	0.93	0.12	31,31,31,31	0
57	MG	1A	3491	1/1	0.93	0.24	57,57,57,57	0
57	MG	2A	3511	1/1	0.93	0.18	55,55,55,55	0
57	MG	1a	1766	1/1	0.93	0.12	50,50,50,50	0
57	MG	1A	3253	1/1	0.93	0.26	49,49,49,49	0
57	MG	1A	4106	1/1	0.93	0.15	43,43,43,43	0
57	MG	2A	3515	1/1	0.93	0.13	47,47,47,47	0
57	MG	1A	4107	1/1	0.93	0.15	65,65,65,65	0
57	MG	1A	3999	1/1	0.93	0.15	24,24,24,24	0
57	MG	1A	3914	1/1	0.93	0.16	62,62,62,62	0
57	MG	2A	3519	1/1	0.93	0.16	59,59,59,59	0
57	MG	1A	3618	1/1	0.93	0.16	53,53,53,53	0
57	MG	1a	1626	1/1	0.93	0.19	52,52,52,52	0
57	MG	1A	3153	1/1	0.93	0.12	37,37,37,37	0
57	MG	1a	1628	1/1	0.93	0.17	61,61,61,61	0
57	MG	1A	3324	1/1	0.93	0.10	38,38,38,38	0
57	MG	1A	4005	1/1	0.93	0.09	38,38,38,38	0
57	MG	1A	3821	1/1	0.93	0.17	28,28,28,28	0
57	MG	1B	217	1/1	0.93	0.22	34,34,34,34	0
57	MG	1a	1635	1/1	0.93	0.14	59,59,59,59	0
57	MG	1B	223	1/1	0.93	0.09	55,55,55,55	0
57	MG	2A	3281	1/1	0.93	0.15	58,58,58,58	0
57	MG	1A	3923	1/1	0.93	0.17	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3400	1/1	0.93	0.20	64,64,64,64	0
57	MG	1a	1641	1/1	0.93	0.23	52,52,52,52	0
57	MG	2A	3096	1/1	0.93	0.19	51,51,51,51	0
57	MG	2A	3097	1/1	0.93	0.09	62,62,62,62	0
57	MG	1a	1800	1/1	0.93	0.13	47,47,47,47	0
57	MG	1A	3356	1/1	0.93	0.20	46,46,46,46	0
57	MG	2A	3101	1/1	0.93	0.10	69,69,69,69	0
57	MG	1A	3829	1/1	0.93	0.10	41,41,41,41	0
57	MG	2A	3553	1/1	0.93	0.13	42,42,42,42	0
57	MG	1a	1644	1/1	0.93	0.13	58,58,58,58	0
57	MG	2A	3303	1/1	0.93	0.25	59,59,59,59	0
57	MG	2A	3104	1/1	0.93	0.25	50,50,50,50	0
57	MG	1A	3835	1/1	0.93	0.15	38,38,38,38	0
57	MG	1B	231	1/1	0.93	0.19	54,54,54,54	0
57	MG	1B	232	1/1	0.93	0.15	43,43,43,43	0
57	MG	1A	3256	1/1	0.93	0.19	66,66,66,66	0
57	MG	2a	1632	1/1	0.93	0.28	60,60,60,60	0
57	MG	1A	3111	1/1	0.93	0.24	33,33,33,33	0
57	MG	2A	3564	1/1	0.93	0.15	56,56,56,56	0
57	MG	2A	3311	1/1	0.93	0.23	56,56,56,56	0
57	MG	1A	3406	1/1	0.93	0.36	51,51,51,51	0
57	MG	2a	1639	1/1	0.93	0.10	53,53,53,53	0
57	MG	1D	312	1/1	0.93	0.20	37,37,37,37	0
57	MG	1A	3296	1/1	0.93	0.09	53,53,53,53	0
57	MG	2a	1643	1/1	0.93	0.32	73,73,73,73	0
57	MG	2A	3118	1/1	0.93	0.16	39,39,39,39	0
57	MG	1a	1658	1/1	0.93	0.28	60,60,60,60	0
57	MG	1A	3456	1/1	0.93	0.16	54,54,54,54	0
57	MG	1A	3188	1/1	0.93	0.47	32,32,32,32	0
57	MG	1A	3643	1/1	0.93	0.18	59,59,59,59	0
57	MG	2a	1651	1/1	0.93	0.38	58,58,58,58	0
57	MG	2a	1653	1/1	0.93	0.17	69,69,69,69	0
57	MG	1a	1821	1/1	0.93	0.09	58,58,58,58	0
57	MG	2A	3332	1/1	0.93	0.10	49,49,49,49	0
57	MG	1A	3644	1/1	0.93	0.18	38,38,38,38	0
57	MG	1A	3939	1/1	0.93	0.14	36,36,36,36	0
57	MG	2A	3130	1/1	0.93	0.17	58,58,58,58	0
57	MG	1a	1826	1/1	0.93	0.14	56,56,56,56	0
57	MG	1A	3848	1/1	0.93	0.14	50,50,50,50	0
57	MG	2A	3134	1/1	0.93	0.28	59,59,59,59	0
57	MG	2A	3136	1/1	0.93	0.25	49,49,49,49	0
57	MG	1A	3458	1/1	0.93	0.15	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3139	1/1	0.93	0.15	37,37,37,37	0
57	MG	1A	3850	1/1	0.93	0.25	56,56,56,56	0
57	MG	2A	3353	1/1	0.93	0.28	61,61,61,61	0
57	MG	1A	3052	1/1	0.93	0.08	46,46,46,46	0
57	MG	1A	3261	1/1	0.93	0.14	62,62,62,62	0
57	MG	1e	201	1/1	0.93	0.17	67,67,67,67	0
57	MG	2A	3603	1/1	0.93	0.07	60,60,60,60	0
57	MG	1a	1671	1/1	0.93	0.31	58,58,58,58	0
57	MG	1A	3070	1/1	0.93	0.40	34,34,34,34	0
57	MG	1A	3136	1/1	0.93	0.17	28,28,28,28	0
57	MG	1A	3465	1/1	0.93	0.20	54,54,54,54	0
57	MG	1A	3575	1/1	0.93	0.16	46,46,46,46	0
57	MG	1n	102	1/1	0.93	0.12	55,55,55,55	0
57	MG	1O	206	1/1	0.93	0.10	64,64,64,64	0
57	MG	2A	3620	1/1	0.93	0.13	43,43,43,43	0
57	MG	1P	203	1/1	0.93	0.16	33,33,33,33	0
57	MG	2A	3162	1/1	0.93	0.22	64,64,64,64	0
57	MG	2A	3623	1/1	0.93	0.10	58,58,58,58	0
57	MG	1A	3137	1/1	0.93	0.25	40,40,40,40	0
57	MG	2a	1691	1/1	0.93	0.18	58,58,58,58	0
57	MG	1a	1682	1/1	0.93	0.88	63,63,63,63	0
57	MG	1A	3660	1/1	0.93	0.17	46,46,46,46	0
57	MG	1A	3582	1/1	0.93	0.53	39,39,39,39	0
57	MG	2a	1695	1/1	0.93	0.23	64,64,64,64	0
57	MG	2A	3375	1/1	0.93	0.32	45,45,45,45	0
57	MG	2A	3169	1/1	0.93	0.13	62,62,62,62	0
57	MG	2A	3382	1/1	0.93	0.12	52,52,52,52	0
57	MG	2A	3383	1/1	0.93	0.16	55,55,55,55	0
57	MG	1a	1686	1/1	0.93	0.06	51,51,51,51	0
57	MG	1a	1687	1/1	0.93	0.22	48,48,48,48	0
57	MG	2A	3394	1/1	0.93	0.15	50,50,50,50	0
57	MG	1A	3095	1/1	0.93	0.10	32,32,32,32	0
57	MG	2a	1708	1/1	0.93	0.10	60,60,60,60	0
57	MG	1A	3584	1/1	0.93	0.21	44,44,44,44	0
57	MG	1S	201	1/1	0.93	0.96	46,46,46,46	0
57	MG	2A	3398	1/1	0.93	0.08	44,44,44,44	0
57	MG	2a	1712	1/1	0.93	0.10	68,68,68,68	0
57	MG	1A	4052	1/1	0.93	0.28	31,31,31,31	0
57	MG	1A	3372	1/1	0.93	0.17	32,32,32,32	0
57	MG	2a	1716	1/1	0.93	0.25	56,56,56,56	0
57	MG	1A	3667	1/1	0.93	0.12	48,48,48,48	0
57	MG	1A	3421	1/1	0.93	0.16	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3652	1/1	0.93	0.08	80,80,80,80	0
57	MG	2A	3181	1/1	0.93	0.24	61,61,61,61	0
57	MG	2A	3654	1/1	0.93	0.22	52,52,52,52	0
57	MG	1A	3877	1/1	0.93	0.09	30,30,30,30	0
57	MG	2A	3657	1/1	0.93	0.09	65,65,65,65	0
57	MG	1A	3337	1/1	0.93	0.26	43,43,43,43	0
57	MG	1W	205	1/1	0.93	0.13	34,34,34,34	0
57	MG	1A	4059	1/1	0.93	0.27	70,70,70,70	0
57	MG	1a	1707	1/1	0.93	0.19	57,57,57,57	0
57	MG	1X	103	1/1	0.93	0.13	51,51,51,51	0
57	MG	1A	3474	1/1	0.93	0.13	52,52,52,52	0
57	MG	2a	1735	1/1	0.93	0.17	61,61,61,61	0
57	MG	1A	3044	1/1	0.93	0.18	38,38,38,38	0
57	MG	1A	4064	1/1	0.93	0.14	68,68,68,68	0
57	MG	2a	1738	1/1	0.93	0.10	57,57,57,57	0
57	MG	1A	3594	1/1	0.93	0.29	43,43,43,43	0
57	MG	1A	3774	1/1	0.93	0.19	28,28,28,28	0
57	MG	1a	1716	1/1	0.93	0.15	57,57,57,57	0
57	MG	2A	3007	1/1	0.93	0.12	53,53,53,53	0
57	MG	1A	3885	1/1	0.93	0.28	39,39,39,39	0
57	MG	1A	3339	1/1	0.93	0.18	54,54,54,54	0
57	MG	2A	3014	1/1	0.93	0.30	45,45,45,45	0
57	MG	2A	3685	1/1	0.93	0.15	46,46,46,46	0
57	MG	1A	3376	1/1	0.93	0.39	58,58,58,58	0
57	MG	2a	1756	1/1	0.93	0.28	73,73,73,73	0
57	MG	1A	3976	1/1	0.93	0.10	54,54,54,54	0
57	MG	2A	3204	1/1	0.93	0.12	48,48,48,48	0
57	MG	1l	101	1/1	0.93	0.56	39,39,39,39	0
57	MG	2A	3443	1/1	0.93	0.14	41,41,41,41	0
57	MG	2A	3444	1/1	0.93	0.18	64,64,64,64	0
57	MG	1A	4076	1/1	0.93	0.23	41,41,41,41	0
57	MG	1a	1724	1/1	0.93	0.14	72,72,72,72	0
57	MG	2A	3447	1/1	0.93	0.10	39,39,39,39	0
57	MG	12	102	1/1	0.93	0.22	43,43,43,43	0
57	MG	1A	4077	1/1	0.93	0.13	31,31,31,31	0
57	MG	1A	3098	1/1	0.93	0.28	58,58,58,58	0
57	MG	1A	3890	1/1	0.93	0.14	45,45,45,45	0
57	MG	2A	3033	1/1	0.93	0.27	56,56,56,56	0
57	MG	2a	1771	1/1	0.93	0.13	61,61,61,61	0
57	MG	2a	1773	1/1	0.93	0.15	64,64,64,64	0
57	MG	2A	3034	1/1	0.93	0.13	40,40,40,40	0
57	MG	15	105	1/1	0.93	0.21	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3712	1/1	0.93	0.12	58,58,58,58	0
57	MG	15	107	1/1	0.93	0.13	31,31,31,31	0
57	MG	2A	3716	1/1	0.93	0.17	60,60,60,60	0
57	MG	2A	3717	1/1	0.93	0.12	57,57,57,57	0
57	MG	1A	3379	1/1	0.93	0.17	52,52,52,52	0
57	MG	1A	3983	1/1	0.93	0.15	50,50,50,50	0
57	MG	2A	3467	1/1	0.93	0.12	40,40,40,40	0
57	MG	2A	3041	1/1	0.93	0.10	63,63,63,63	0
57	MG	2A	3728	1/1	0.93	0.22	51,51,51,51	0
57	MG	18	3401	1/1	0.93	0.40	54,54,54,54	0
57	MG	1A	3100	1/1	0.93	0.10	61,61,61,61	0
57	MG	1a	1742	1/1	0.93	0.22	56,56,56,56	0
57	MG	1A	3603	1/1	0.93	0.22	47,47,47,47	0
57	MG	2A	3234	1/1	0.93	0.09	61,61,61,61	0
57	MG	1A	4089	1/1	0.93	0.18	53,53,53,53	0
57	MG	1a	1601	1/1	0.93	0.10	66,66,66,66	0
57	MG	2B	208	1/1	0.93	0.23	62,62,62,62	0
57	MG	1A	3386	1/1	0.93	0.13	24,24,24,24	0
57	MG	2y	101	1/1	0.93	0.23	56,56,56,56	0
57	MG	2y	103	1/1	0.93	0.28	58,58,58,58	0
57	MG	1A	4092	1/1	0.93	0.12	63,63,63,63	0
57	MG	1A	3387	1/1	0.93	0.20	35,35,35,35	0
57	MG	1A	3091	1/1	0.93	0.20	25,25,25,25	0
57	MG	2A	3492	1/1	0.93	0.10	56,56,56,56	0
57	MG	2B	215	1/1	0.94	0.22	65,65,65,65	0
57	MG	2A	3490	1/1	0.94	0.21	48,48,48,48	0
57	MG	1a	1772	1/1	0.94	0.14	68,68,68,68	0
57	MG	1B	227	1/1	0.94	0.16	53,53,53,53	0
57	MG	2D	301	1/1	0.94	0.19	55,55,55,55	0
57	MG	2D	303	1/1	0.94	0.18	51,51,51,51	0
57	MG	1A	3139	1/1	0.94	0.12	39,39,39,39	0
57	MG	1A	3905	1/1	0.94	0.10	43,43,43,43	0
57	MG	2E	304	1/1	0.94	0.10	57,57,57,57	0
57	MG	1A	3796	1/1	0.94	0.11	29,29,29,29	0
57	MG	2A	3497	1/1	0.94	0.13	58,58,58,58	0
57	MG	1a	1631	1/1	0.94	0.12	62,62,62,62	0
57	MG	2F	305	1/1	0.94	0.52	47,47,47,47	0
57	MG	2A	3499	1/1	0.94	0.22	55,55,55,55	0
57	MG	1A	3909	1/1	0.94	0.12	54,54,54,54	0
57	MG	2N	201	1/1	0.94	0.18	57,57,57,57	0
57	MG	1A	3697	1/1	0.94	0.20	25,25,25,25	0
57	MG	1A	3803	1/1	0.94	0.11	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3078	1/1	0.94	0.29	41,41,41,41	0
57	MG	1a	1785	1/1	0.94	0.18	50,50,50,50	0
57	MG	2A	3509	1/1	0.94	0.19	41,41,41,41	0
57	MG	2A	3510	1/1	0.94	0.16	39,39,39,39	0
57	MG	2A	3080	1/1	0.94	0.20	45,45,45,45	0
57	MG	1a	1636	1/1	0.94	0.24	76,76,76,76	0
57	MG	2A	3262	1/1	0.94	0.21	47,47,47,47	0
57	MG	2A	3263	1/1	0.94	0.27	72,72,72,72	0
57	MG	2A	3264	1/1	0.94	0.16	64,64,64,64	0
57	MG	1A	3805	1/1	0.94	0.16	19,19,19,19	0
57	MG	25	103	1/1	0.94	0.21	56,56,56,56	0
57	MG	1A	3808	1/1	0.94	0.23	20,20,20,20	0
57	MG	2A	3086	1/1	0.94	0.12	34,34,34,34	0
57	MG	27	103	1/1	0.94	0.12	40,40,40,40	0
57	MG	28	101	1/1	0.94	0.13	46,46,46,46	0
57	MG	1a	1639	1/1	0.94	0.17	43,43,43,43	0
57	MG	2A	3270	1/1	0.94	0.22	49,49,49,49	0
57	MG	1D	305	1/1	0.94	0.22	35,35,35,35	0
57	MG	2A	3523	1/1	0.94	0.15	60,60,60,60	0
57	MG	1D	309	1/1	0.94	0.12	42,42,42,42	0
57	MG	1A	3415	1/1	0.94	0.26	63,63,63,63	0
57	MG	1a	1794	1/1	0.94	0.09	56,56,56,56	0
57	MG	2a	1607	1/1	0.94	0.22	69,69,69,69	0
57	MG	2A	3278	1/1	0.94	0.14	60,60,60,60	0
57	MG	1A	3142	1/1	0.94	0.15	38,38,38,38	0
57	MG	1A	3921	1/1	0.94	0.25	36,36,36,36	0
57	MG	1E	304	1/1	0.94	0.18	34,34,34,34	0
57	MG	1a	1646	1/1	0.94	0.09	63,63,63,63	0
57	MG	1A	3417	1/1	0.94	0.15	48,48,48,48	0
57	MG	2A	3538	1/1	0.94	0.15	58,58,58,58	0
57	MG	1a	1648	1/1	0.94	0.10	49,49,49,49	0
57	MG	1E	310	1/1	0.94	0.12	69,69,69,69	0
57	MG	1A	3039	1/1	0.94	0.30	56,56,56,56	0
57	MG	1A	3704	1/1	0.94	0.24	21,21,21,21	0
57	MG	2A	3294	1/1	0.94	0.21	51,51,51,51	0
57	MG	1a	1652	1/1	0.94	0.12	45,45,45,45	0
57	MG	2A	3547	1/1	0.94	0.17	55,55,55,55	0
57	MG	2A	3296	1/1	0.94	0.17	54,54,54,54	0
57	MG	2A	3297	1/1	0.94	0.36	56,56,56,56	0
57	MG	1a	1812	1/1	0.94	0.12	62,62,62,62	0
57	MG	1E	315	1/1	0.94	0.10	59,59,59,59	0
57	MG	2A	3109	1/1	0.94	0.17	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1F	304	1/1	0.94	0.18	31,31,31,31	0
57	MG	1A	3928	1/1	0.94	0.10	54,54,54,54	0
57	MG	1A	3329	1/1	0.94	0.19	53,53,53,53	0
57	MG	1F	311	1/1	0.94	0.18	51,51,51,51	0
57	MG	1A	3007	1/1	0.94	0.17	39,39,39,39	0
57	MG	2A	3117	1/1	0.94	0.29	52,52,52,52	0
57	MG	1A	3822	1/1	0.94	0.13	42,42,42,42	0
57	MG	2A	3310	1/1	0.94	0.24	53,53,53,53	0
57	MG	2a	1642	1/1	0.94	0.11	59,59,59,59	0
57	MG	1A	3823	1/1	0.94	0.09	61,61,61,61	0
57	MG	2A	3312	1/1	0.94	0.14	69,69,69,69	0
57	MG	1A	3184	1/1	0.94	0.21	36,36,36,36	0
57	MG	1N	201	1/1	0.94	0.39	51,51,51,51	0
57	MG	2A	3124	1/1	0.94	0.15	62,62,62,62	0
57	MG	1N	202	1/1	0.94	0.16	46,46,46,46	0
57	MG	1N	204	1/1	0.94	0.28	51,51,51,51	0
57	MG	1A	3288	1/1	0.94	0.25	46,46,46,46	0
57	MG	2A	3578	1/1	0.94	0.15	28,28,28,28	0
57	MG	1A	3074	1/1	0.94	0.15	28,28,28,28	0
57	MG	2A	3129	1/1	0.94	0.15	58,58,58,58	0
57	MG	2A	3325	1/1	0.94	0.24	54,54,54,54	0
57	MG	2A	3328	1/1	0.94	0.22	38,38,38,38	0
57	MG	1A	3830	1/1	0.94	0.08	32,32,32,32	0
57	MG	2A	3331	1/1	0.94	0.17	25,25,25,25	0
57	MG	1A	3833	1/1	0.94	0.10	31,31,31,31	0
57	MG	2A	3334	1/1	0.94	0.23	55,55,55,55	0
57	MG	1O	205	1/1	0.94	0.11	66,66,66,66	0
57	MG	1A	3426	1/1	0.94	0.12	60,60,60,60	0
57	MG	1A	4047	1/1	0.94	0.17	27,27,27,27	0
57	MG	2A	3594	1/1	0.94	0.09	66,66,66,66	0
57	MG	2A	3137	1/1	0.94	0.27	58,58,58,58	0
57	MG	1A	3027	1/1	0.94	0.14	69,69,69,69	0
57	MG	1A	3838	1/1	0.94	0.21	43,43,43,43	0
57	MG	2A	3140	1/1	0.94	0.28	63,63,63,63	0
57	MG	1A	3377	1/1	0.94	0.40	58,58,58,58	0
57	MG	1A	3190	1/1	0.94	0.11	33,33,33,33	0
57	MG	2a	1675	1/1	0.94	0.23	63,63,63,63	0
57	MG	2A	3146	1/1	0.94	0.22	56,56,56,56	0
57	MG	2A	3352	1/1	0.94	0.09	56,56,56,56	0
57	MG	2A	3606	1/1	0.94	0.11	74,74,74,74	0
57	MG	1A	3431	1/1	0.94	0.11	42,42,42,42	0
57	MG	1A	3294	1/1	0.94	0.13	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3610	1/1	0.94	0.08	62,62,62,62	0
57	MG	2a	1685	1/1	0.94	0.17	67,67,67,67	0
57	MG	2a	1686	1/1	0.94	0.08	69,69,69,69	0
57	MG	1A	3383	1/1	0.94	0.11	53,53,53,53	0
57	MG	1A	3119	1/1	0.94	0.17	40,40,40,40	0
57	MG	1T	201	1/1	0.94	0.10	56,56,56,56	0
57	MG	1T	202	1/1	0.94	0.10	51,51,51,51	0
57	MG	1A	3385	1/1	0.94	0.22	34,34,34,34	0
57	MG	2A	3361	1/1	0.94	0.11	55,55,55,55	0
57	MG	1A	3083	1/1	0.94	0.26	38,38,38,38	0
57	MG	1A	3494	1/1	0.94	0.16	41,41,41,41	0
57	MG	2A	3159	1/1	0.94	0.10	54,54,54,54	0
57	MG	1V	205	1/1	0.94	0.28	41,41,41,41	0
57	MG	2A	3626	1/1	0.94	0.07	66,66,66,66	0
57	MG	1A	3646	1/1	0.94	0.07	54,54,54,54	0
57	MG	2A	3163	1/1	0.94	0.18	56,56,56,56	0
57	MG	1W	204	1/1	0.94	0.15	35,35,35,35	0
57	MG	1A	3739	1/1	0.94	0.18	50,50,50,50	0
57	MG	1x	107	1/1	0.94	0.18	51,51,51,51	0
57	MG	1A	3647	1/1	0.94	0.13	35,35,35,35	0
57	MG	1a	1704	1/1	0.94	0.19	52,52,52,52	0
57	MG	1X	102	1/1	0.94	0.23	27,27,27,27	0
57	MG	2A	3379	1/1	0.94	0.18	38,38,38,38	0
57	MG	2A	3639	1/1	0.94	0.10	65,65,65,65	0
57	MG	1A	4066	1/1	0.94	0.17	46,46,46,46	0
57	MG	2A	3641	1/1	0.94	0.12	52,52,52,52	0
57	MG	1A	3205	1/1	0.94	0.08	59,59,59,59	0
57	MG	1A	3206	1/1	0.94	0.21	34,34,34,34	0
57	MG	1A	3497	1/1	0.94	0.12	35,35,35,35	0
57	MG	2a	1718	1/1	0.94	0.15	65,65,65,65	0
57	MG	1A	3048	1/1	0.94	0.15	16,16,16,16	0
57	MG	1A	3157	1/1	0.94	0.21	34,34,34,34	0
57	MG	1A	3750	1/1	0.94	0.15	52,52,52,52	0
57	MG	1A	3751	1/1	0.94	0.14	45,45,45,45	0
57	MG	1A	3087	1/1	0.94	0.23	48,48,48,48	0
57	MG	2a	1726	1/1	0.94	0.15	68,68,68,68	0
57	MG	1A	3101	1/1	0.94	0.11	33,33,33,33	0
57	MG	1A	3871	1/1	0.94	0.10	35,35,35,35	0
57	MG	1A	3397	1/1	0.94	0.31	42,42,42,42	0
57	MG	1A	3873	1/1	0.94	0.17	40,40,40,40	0
57	MG	2A	3009	1/1	0.94	0.12	45,45,45,45	0
57	MG	1a	1722	1/1	0.94	0.12	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3449	1/1	0.94	0.19	41,41,41,41	0
57	MG	2A	3412	1/1	0.94	0.13	43,43,43,43	0
57	MG	2A	3191	1/1	0.94	0.20	36,36,36,36	0
57	MG	2A	3664	1/1	0.94	0.11	48,48,48,48	0
57	MG	1A	3581	1/1	0.94	0.23	30,30,30,30	0
57	MG	1A	3129	1/1	0.94	0.23	31,31,31,31	0
57	MG	1a	1726	1/1	0.94	0.09	53,53,53,53	0
57	MG	2a	1741	1/1	0.94	0.22	45,45,45,45	0
57	MG	2A	3020	1/1	0.94	0.23	51,51,51,51	0
57	MG	2A	3674	1/1	0.94	0.08	50,50,50,50	0
57	MG	2a	1745	1/1	0.94	0.13	49,49,49,49	0
57	MG	2A	3675	1/1	0.94	0.13	37,37,37,37	0
57	MG	2a	1749	1/1	0.94	0.23	68,68,68,68	0
57	MG	2a	1750	1/1	0.94	0.21	55,55,55,55	0
57	MG	14	101	1/1	0.94	0.15	64,64,64,64	0
57	MG	1A	3979	1/1	0.94	0.17	27,27,27,27	0
57	MG	2A	3425	1/1	0.94	0.22	43,43,43,43	0
57	MG	1A	3347	1/1	0.94	0.08	60,60,60,60	0
57	MG	1A	3762	1/1	0.94	0.10	40,40,40,40	0
57	MG	1A	3025	1/1	0.94	0.14	34,34,34,34	0
57	MG	1A	3104	1/1	0.94	0.16	36,36,36,36	0
57	MG	1A	3262	1/1	0.94	0.11	57,57,57,57	0
57	MG	2A	3688	1/1	0.94	0.07	59,59,59,59	0
57	MG	1A	3065	1/1	0.94	0.20	36,36,36,36	0
57	MG	2A	3036	1/1	0.94	0.14	52,52,52,52	0
57	MG	2a	1763	1/1	0.94	0.12	64,64,64,64	0
57	MG	2A	3206	1/1	0.94	0.12	44,44,44,44	0
57	MG	1a	1740	1/1	0.94	0.14	57,57,57,57	0
57	MG	2A	3439	1/1	0.94	0.14	51,51,51,51	0
57	MG	1A	3135	1/1	0.94	0.15	49,49,49,49	0
57	MG	19	101	1/1	0.94	0.18	44,44,44,44	0
57	MG	1A	3773	1/1	0.94	0.17	31,31,31,31	0
57	MG	2A	3213	1/1	0.94	0.17	57,57,57,57	0
57	MG	2A	3702	1/1	0.94	0.14	44,44,44,44	0
57	MG	2a	1772	1/1	0.94	0.13	57,57,57,57	0
57	MG	1A	3220	1/1	0.94	0.21	40,40,40,40	0
57	MG	2A	3215	1/1	0.94	0.14	54,54,54,54	0
57	MG	1A	3067	1/1	0.94	0.11	48,48,48,48	0
57	MG	1A	4108	1/1	0.94	0.12	54,54,54,54	0
57	MG	2A	3044	1/1	0.94	0.07	52,52,52,52	0
57	MG	1A	3685	1/1	0.94	0.21	21,21,21,21	0
57	MG	1A	3892	1/1	0.94	0.21	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3270	1/1	0.94	0.17	35,35,35,35	0
57	MG	1B	205	1/1	0.94	0.14	44,44,44,44	0
57	MG	1A	3462	1/1	0.94	0.15	61,61,61,61	0
57	MG	1A	3780	1/1	0.94	0.18	28,28,28,28	0
57	MG	2e	201	1/1	0.94	0.10	72,72,72,72	0
57	MG	1A	3898	1/1	0.94	0.10	43,43,43,43	0
57	MG	1A	3112	1/1	0.94	0.20	33,33,33,33	0
57	MG	1B	216	1/1	0.94	0.27	38,38,38,38	0
57	MG	2q	201	1/1	0.94	0.12	67,67,67,67	0
57	MG	2A	3468	1/1	0.94	0.21	67,67,67,67	0
57	MG	2A	3233	1/1	0.94	0.12	57,57,57,57	0
57	MG	1A	3464	1/1	0.94	0.21	48,48,48,48	0
57	MG	1B	221	1/1	0.94	0.22	57,57,57,57	0
57	MG	2A	3474	1/1	0.94	0.18	56,56,56,56	0
57	MG	2A	3060	1/1	0.94	0.20	58,58,58,58	0
57	MG	1a	1764	1/1	0.94	0.14	54,54,54,54	0
57	MG	1a	1765	1/1	0.94	0.05	61,61,61,61	0
57	MG	2y	102	1/1	0.94	0.07	81,81,81,81	0
57	MG	1A	3226	1/1	0.94	0.16	37,37,37,37	0
57	MG	2A	3242	1/1	0.94	0.51	67,67,67,67	0
57	MG	1a	1767	1/1	0.94	0.11	64,64,64,64	0
57	MG	1A	3693	1/1	0.94	0.19	22,22,22,22	0
57	MG	1A	3413	1/1	0.94	0.22	33,33,33,33	0
57	MG	1A	3571	1/1	0.95	0.22	28,28,28,28	0
57	MG	1A	3359	1/1	0.95	0.26	62,62,62,62	0
57	MG	1B	210	1/1	0.95	0.49	55,55,55,55	0
57	MG	1B	211	1/1	0.95	0.14	50,50,50,50	0
57	MG	1A	3159	1/1	0.95	0.23	29,29,29,29	0
57	MG	1B	213	1/1	0.95	0.22	42,42,42,42	0
57	MG	1B	214	1/1	0.95	0.20	44,44,44,44	0
57	MG	2T	201	1/1	0.95	0.24	53,53,53,53	0
57	MG	2A	3081	1/1	0.95	0.16	34,34,34,34	0
57	MG	1A	3227	1/1	0.95	0.21	36,36,36,36	0
57	MG	1a	1619	1/1	0.95	0.09	54,54,54,54	0
57	MG	1A	3510	1/1	0.95	0.18	69,69,69,69	0
57	MG	1B	219	1/1	0.95	0.24	45,45,45,45	0
57	MG	1A	3363	1/1	0.95	0.32	63,63,63,63	0
57	MG	1A	3763	1/1	0.95	0.20	41,41,41,41	0
57	MG	2A	3089	1/1	0.95	0.18	46,46,46,46	0
57	MG	2A	3282	1/1	0.95	0.21	51,51,51,51	0
57	MG	1A	3884	1/1	0.95	0.18	32,32,32,32	0
57	MG	2A	3530	1/1	0.95	0.10	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1B	225	1/1	0.95	0.20	36,36,36,36	0
57	MG	2A	3093	1/1	0.95	0.25	57,57,57,57	0
57	MG	1A	3996	1/1	0.95	0.23	26,26,26,26	0
57	MG	2A	3291	1/1	0.95	0.31	48,48,48,48	0
57	MG	1A	3580	1/1	0.95	0.37	40,40,40,40	0
57	MG	1A	3512	1/1	0.95	0.14	46,46,46,46	0
57	MG	1A	3668	1/1	0.95	0.18	36,36,36,36	0
57	MG	1a	1790	1/1	0.95	0.11	73,73,73,73	0
57	MG	2A	3099	1/1	0.95	0.16	50,50,50,50	0
57	MG	2a	1605	1/1	0.95	0.11	58,58,58,58	0
57	MG	1A	4001	1/1	0.95	0.17	28,28,28,28	0
57	MG	1A	3769	1/1	0.95	0.17	16,16,16,16	0
57	MG	1A	3513	1/1	0.95	0.20	46,46,46,46	0
57	MG	2A	3301	1/1	0.95	0.15	57,57,57,57	0
57	MG	1A	3671	1/1	0.95	0.20	24,24,24,24	0
57	MG	1a	1795	1/1	0.95	0.33	74,74,74,74	0
57	MG	2A	3105	1/1	0.95	0.14	48,48,48,48	0
57	MG	1a	1796	1/1	0.95	0.21	45,45,45,45	0
57	MG	1A	3672	1/1	0.95	0.23	23,23,23,23	0
57	MG	1a	1799	1/1	0.95	0.12	55,55,55,55	0
57	MG	1A	3017	1/1	0.95	0.18	60,60,60,60	0
57	MG	1D	302	1/1	0.95	0.34	43,43,43,43	0
57	MG	1D	303	1/1	0.95	0.13	40,40,40,40	0
57	MG	2A	3112	1/1	0.95	0.26	42,42,42,42	0
57	MG	1A	3894	1/1	0.95	0.17	27,27,27,27	0
57	MG	1D	308	1/1	0.95	0.20	48,48,48,48	0
57	MG	1a	1807	1/1	0.95	0.09	60,60,60,60	0
57	MG	1A	3516	1/1	0.95	0.20	35,35,35,35	0
57	MG	1D	311	1/1	0.95	0.14	52,52,52,52	0
57	MG	1A	3776	1/1	0.95	0.19	28,28,28,28	0
57	MG	1A	3517	1/1	0.95	0.16	50,50,50,50	0
57	MG	1A	3678	1/1	0.95	0.14	22,22,22,22	0
57	MG	1A	3103	1/1	0.95	0.16	46,46,46,46	0
57	MG	1A	3680	1/1	0.95	0.12	34,34,34,34	0
57	MG	2A	3573	1/1	0.95	0.14	57,57,57,57	0
57	MG	1E	307	1/1	0.95	0.34	49,49,49,49	0
57	MG	1A	3193	1/1	0.95	0.35	37,37,37,37	0
57	MG	1E	312	1/1	0.95	0.17	25,25,25,25	0
57	MG	1A	3194	1/1	0.95	0.37	36,36,36,36	0
57	MG	1a	1654	1/1	0.95	0.11	42,42,42,42	0
57	MG	2A	3336	1/1	0.95	0.67	49,49,49,49	0
57	MG	1A	3198	1/1	0.95	0.14	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1a	1656	1/1	0.95	0.10	43,43,43,43	0
57	MG	2A	3339	1/1	0.95	0.06	56,56,56,56	0
57	MG	1A	3523	1/1	0.95	0.20	34,34,34,34	0
57	MG	1a	1825	1/1	0.95	0.19	49,49,49,49	0
57	MG	1A	3789	1/1	0.95	0.15	25,25,25,25	0
57	MG	2a	1652	1/1	0.95	0.09	55,55,55,55	0
57	MG	1A	3120	1/1	0.95	0.36	42,42,42,42	0
57	MG	2A	3344	1/1	0.95	0.10	53,53,53,53	0
57	MG	1a	1828	1/1	0.95	0.21	59,59,59,59	0
57	MG	1A	3793	1/1	0.95	0.20	25,25,25,25	0
57	MG	2A	3141	1/1	0.95	0.28	54,54,54,54	0
57	MG	1a	1661	1/1	0.95	0.21	50,50,50,50	0
57	MG	2A	3599	1/1	0.95	0.09	36,36,36,36	0
57	MG	1A	3370	1/1	0.95	0.34	51,51,51,51	0
57	MG	1A	3243	1/1	0.95	0.17	42,42,42,42	0
57	MG	1G	201	1/1	0.95	0.21	39,39,39,39	0
57	MG	2a	1664	1/1	0.95	0.08	55,55,55,55	0
57	MG	1G	202	1/1	0.95	0.17	56,56,56,56	0
57	MG	1A	4034	1/1	0.95	0.13	52,52,52,52	0
57	MG	1A	3244	1/1	0.95	0.09	37,37,37,37	0
57	MG	1A	4036	1/1	0.95	0.18	44,44,44,44	0
57	MG	2A	3153	1/1	0.95	0.22	57,57,57,57	0
57	MG	1A	3053	1/1	0.95	0.11	37,37,37,37	0
57	MG	1A	3804	1/1	0.95	0.08	36,36,36,36	0
57	MG	1A	3105	1/1	0.95	0.20	30,30,30,30	0
57	MG	2A	3616	1/1	0.95	0.17	42,42,42,42	0
57	MG	1A	3125	1/1	0.95	0.32	28,28,28,28	0
57	MG	1A	3291	1/1	0.95	0.28	53,53,53,53	0
57	MG	1O	202	1/1	0.95	0.42	53,53,53,53	0
57	MG	2a	1678	1/1	0.95	0.11	76,76,76,76	0
57	MG	2A	3161	1/1	0.95	0.29	55,55,55,55	0
57	MG	1A	3248	1/1	0.95	0.16	57,57,57,57	0
57	MG	1A	3702	1/1	0.95	0.15	26,26,26,26	0
57	MG	1a	1679	1/1	0.95	0.14	60,60,60,60	0
57	MG	1a	1680	1/1	0.95	0.06	70,70,70,70	0
57	MG	1x	101	1/1	0.95	0.09	47,47,47,47	0
57	MG	1A	3812	1/1	0.95	0.09	40,40,40,40	0
57	MG	1A	3536	1/1	0.95	0.14	48,48,48,48	0
57	MG	2A	3629	1/1	0.95	0.19	49,49,49,49	0
57	MG	2A	3380	1/1	0.95	0.12	54,54,54,54	0
57	MG	1A	3816	1/1	0.95	0.09	36,36,36,36	0
57	MG	2A	3171	1/1	0.95	0.26	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3817	1/1	0.95	0.14	25,25,25,25	0
57	MG	1A	3171	1/1	0.95	0.41	41,41,41,41	0
57	MG	2A	3387	1/1	0.95	0.11	36,36,36,36	0
57	MG	2A	3388	1/1	0.95	0.19	53,53,53,53	0
57	MG	2A	3392	1/1	0.95	0.12	58,58,58,58	0
57	MG	2a	1697	1/1	0.95	0.12	51,51,51,51	0
57	MG	1A	3145	1/1	0.95	0.21	29,29,29,29	0
57	MG	1a	1689	1/1	0.95	0.16	60,60,60,60	0
57	MG	1A	3073	1/1	0.95	0.23	21,21,21,21	0
57	MG	1A	3177	1/1	0.95	0.23	19,19,19,19	0
57	MG	2A	3644	1/1	0.95	0.10	54,54,54,54	0
57	MG	1R	203	1/1	0.95	0.12	42,42,42,42	0
57	MG	2a	1706	1/1	0.95	0.09	71,71,71,71	0
57	MG	1R	204	1/1	0.95	0.23	36,36,36,36	0
57	MG	1A	3710	1/1	0.95	0.16	57,57,57,57	0
57	MG	2A	3402	1/1	0.95	0.09	36,36,36,36	0
57	MG	1a	1695	1/1	0.95	0.09	64,64,64,64	0
57	MG	1A	3711	1/1	0.95	0.21	30,30,30,30	0
57	MG	1A	3713	1/1	0.95	0.14	14,14,14,14	0
57	MG	1A	3940	1/1	0.95	0.14	35,35,35,35	0
57	MG	1a	1701	1/1	0.95	0.29	47,47,47,47	0
57	MG	2A	3002	1/1	0.95	0.30	58,58,58,58	0
57	MG	1A	4060	1/1	0.95	0.14	17,17,17,17	0
57	MG	1A	3616	1/1	0.95	0.11	40,40,40,40	0
57	MG	1A	3715	1/1	0.95	0.14	25,25,25,25	0
57	MG	1a	1705	1/1	0.95	0.19	49,49,49,49	0
57	MG	2a	1721	1/1	0.95	0.25	47,47,47,47	0
57	MG	1A	3028	1/1	0.95	0.24	39,39,39,39	0
57	MG	1V	204	1/1	0.95	0.15	30,30,30,30	0
57	MG	1A	3075	1/1	0.95	0.19	42,42,42,42	0
57	MG	1A	3303	1/1	0.95	0.31	38,38,38,38	0
57	MG	1A	3217	1/1	0.95	0.14	46,46,46,46	0
57	MG	2A	3670	1/1	0.95	0.12	38,38,38,38	0
57	MG	2A	3671	1/1	0.95	0.10	53,53,53,53	0
57	MG	1a	1711	1/1	0.95	0.25	57,57,57,57	0
57	MG	1A	3306	1/1	0.95	0.25	44,44,44,44	0
57	MG	2A	3430	1/1	0.95	0.17	34,34,34,34	0
57	MG	1A	3723	1/1	0.95	0.07	56,56,56,56	0
57	MG	1A	3628	1/1	0.95	0.25	32,32,32,32	0
57	MG	1A	3726	1/1	0.95	0.27	56,56,56,56	0
57	MG	1A	3630	1/1	0.95	0.20	23,23,23,23	0
57	MG	2A	3024	1/1	0.95	0.14	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3683	1/1	0.95	0.15	47,47,47,47	0
57	MG	2A	3207	1/1	0.95	0.17	56,56,56,56	0
57	MG	1A	3729	1/1	0.95	0.23	44,44,44,44	0
57	MG	1A	3099	1/1	0.95	0.14	33,33,33,33	0
57	MG	1A	3392	1/1	0.95	0.29	37,37,37,37	0
57	MG	2A	3029	1/1	0.95	0.11	54,54,54,54	0
57	MG	2a	1746	1/1	0.95	0.22	58,58,58,58	0
57	MG	2A	3030	1/1	0.95	0.14	50,50,50,50	0
57	MG	2A	3031	1/1	0.95	0.11	53,53,53,53	0
57	MG	2A	3032	1/1	0.95	0.11	33,33,33,33	0
57	MG	2A	3694	1/1	0.95	0.11	41,41,41,41	0
57	MG	2a	1752	1/1	0.95	0.35	52,52,52,52	0
57	MG	1A	3636	1/1	0.95	0.23	24,24,24,24	0
57	MG	10	101	1/1	0.95	0.15	38,38,38,38	0
57	MG	1A	3393	1/1	0.95	0.35	44,44,44,44	0
57	MG	1A	3551	1/1	0.95	0.22	17,17,17,17	0
57	MG	2A	3222	1/1	0.95	0.11	60,60,60,60	0
57	MG	1A	3442	1/1	0.95	0.24	46,46,46,46	0
57	MG	1A	3854	1/1	0.95	0.14	51,51,51,51	0
57	MG	2A	3705	1/1	0.95	0.29	59,59,59,59	0
57	MG	2A	3457	1/1	0.95	0.12	53,53,53,53	0
57	MG	2A	3459	1/1	0.95	0.12	41,41,41,41	0
57	MG	1A	3737	1/1	0.95	0.06	52,52,52,52	0
57	MG	11	102	1/1	0.95	0.12	49,49,49,49	0
57	MG	1A	3015	1/1	0.95	0.18	41,41,41,41	0
57	MG	2A	3465	1/1	0.95	0.10	43,43,43,43	0
57	MG	2A	3229	1/1	0.95	0.08	60,60,60,60	0
57	MG	11	105	1/1	0.95	0.21	68,68,68,68	0
57	MG	1A	3742	1/1	0.95	0.19	23,23,23,23	0
57	MG	13	101	1/1	0.95	0.21	36,36,36,36	0
57	MG	1A	3260	1/1	0.95	0.15	53,53,53,53	0
57	MG	1A	3971	1/1	0.95	0.14	43,43,43,43	0
57	MG	1A	3080	1/1	0.95	0.20	38,38,38,38	0
57	MG	2A	3475	1/1	0.95	0.24	58,58,58,58	0
57	MG	1A	4097	1/1	0.95	0.15	64,64,64,64	0
57	MG	1A	3185	1/1	0.95	0.21	39,39,39,39	0
57	MG	1A	4099	1/1	0.95	0.29	53,53,53,53	0
57	MG	2A	3054	1/1	0.95	0.20	51,51,51,51	0
57	MG	1A	3974	1/1	0.95	0.10	24,24,24,24	0
57	MG	16	101	1/1	0.95	0.13	47,47,47,47	0
57	MG	2A	3057	1/1	0.95	0.13	61,61,61,61	0
57	MG	2B	207	1/1	0.95	0.18	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3866	1/1	0.95	0.20	34,34,34,34	0
57	MG	2B	209	1/1	0.95	0.25	65,65,65,65	0
57	MG	2A	3489	1/1	0.95	0.11	43,43,43,43	0
57	MG	2f	202	1/1	0.95	0.16	73,73,73,73	0
57	MG	17	105	1/1	0.95	0.10	54,54,54,54	0
57	MG	17	106	1/1	0.95	0.16	43,43,43,43	0
57	MG	1A	3498	1/1	0.95	0.41	55,55,55,55	0
57	MG	1A	4105	1/1	0.95	0.16	47,47,47,47	0
57	MG	1a	1755	1/1	0.95	0.12	43,43,43,43	0
57	MG	2r	101	1/1	0.95	0.12	61,61,61,61	0
57	MG	1A	3352	1/1	0.95	0.20	49,49,49,49	0
57	MG	2w	101	1/1	0.95	0.12	55,55,55,55	0
57	MG	1A	3353	1/1	0.95	0.17	28,28,28,28	0
57	MG	1A	3223	1/1	0.95	0.12	47,47,47,47	0
57	MG	2D	302	1/1	0.95	0.37	44,44,44,44	0
57	MG	1A	3117	1/1	0.95	0.18	28,28,28,28	0
57	MG	1A	3317	1/1	0.95	0.18	42,42,42,42	0
57	MG	2E	302	1/1	0.95	0.10	66,66,66,66	0
57	MG	1A	3984	1/1	0.95	0.13	56,56,56,56	0
57	MG	2A	3070	1/1	0.95	0.10	46,46,46,46	0
57	MG	2A	3505	1/1	0.95	0.17	35,35,35,35	0
59	ZN	26	102	1/1	0.95	0.21	68,68,68,68	0
57	MG	1A	3568	1/1	0.95	0.17	34,34,34,34	0
57	MG	1A	3875	1/1	0.95	0.14	24,24,24,24	0
57	MG	1A	3141	1/1	0.96	0.20	20,20,20,20	0
57	MG	1A	3293	1/1	0.96	0.25	31,31,31,31	0
57	MG	1A	3443	1/1	0.96	0.24	52,52,52,52	0
57	MG	2A	3522	1/1	0.96	0.25	66,66,66,66	0
57	MG	1A	3042	1/1	0.96	0.33	30,30,30,30	0
57	MG	1P	201	1/1	0.96	0.15	30,30,30,30	0
57	MG	1A	3504	1/1	0.96	0.12	32,32,32,32	0
57	MG	1A	3054	1/1	0.96	0.25	35,35,35,35	0
57	MG	1P	206	1/1	0.96	0.19	50,50,50,50	0
57	MG	1A	3951	1/1	0.96	0.16	38,38,38,38	0
57	MG	1A	3741	1/1	0.96	0.20	26,26,26,26	0
57	MG	1Q	205	1/1	0.96	0.14	40,40,40,40	0
57	MG	2Y	201	1/1	0.96	0.24	44,44,44,44	0
57	MG	2A	3534	1/1	0.96	0.22	60,60,60,60	0
57	MG	1A	3564	1/1	0.96	0.11	23,23,23,23	0
57	MG	1l	203	1/1	0.96	0.12	62,62,62,62	0
57	MG	1A	3954	1/1	0.96	0.07	40,40,40,40	0
57	MG	23	101	1/1	0.96	0.18	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1R	202	1/1	0.96	0.24	46,46,46,46	0
57	MG	1A	3567	1/1	0.96	0.25	31,31,31,31	0
57	MG	1A	4068	1/1	0.96	0.14	25,25,25,25	0
57	MG	1A	3744	1/1	0.96	0.14	49,49,49,49	0
57	MG	1A	3394	1/1	0.96	0.19	24,24,24,24	0
57	MG	27	102	1/1	0.96	0.14	46,46,46,46	0
57	MG	1A	3043	1/1	0.96	0.14	34,34,34,34	0
57	MG	2A	3142	1/1	0.96	0.07	51,51,51,51	0
57	MG	1A	3656	1/1	0.96	0.20	30,30,30,30	0
57	MG	2A	3548	1/1	0.96	0.12	57,57,57,57	0
57	MG	2A	3549	1/1	0.96	0.09	66,66,66,66	0
57	MG	1A	3249	1/1	0.96	0.26	34,34,34,34	0
57	MG	2A	3326	1/1	0.96	0.20	65,65,65,65	0
57	MG	1a	1688	1/1	0.96	0.10	64,64,64,64	0
57	MG	1U	201	1/1	0.96	0.16	30,30,30,30	0
57	MG	2A	3148	1/1	0.96	0.22	37,37,37,37	0
57	MG	1A	3346	1/1	0.96	0.27	41,41,41,41	0
57	MG	2A	3333	1/1	0.96	0.08	62,62,62,62	0
57	MG	1U	208	1/1	0.96	0.21	30,30,30,30	0
57	MG	1A	3173	1/1	0.96	0.19	29,29,29,29	0
57	MG	1A	4079	1/1	0.96	0.21	55,55,55,55	0
57	MG	1A	3299	1/1	0.96	0.13	30,30,30,30	0
57	MG	1A	3123	1/1	0.96	0.14	31,31,31,31	0
57	MG	2a	1615	1/1	0.96	0.13	58,58,58,58	0
57	MG	1A	3858	1/1	0.96	0.09	52,52,52,52	0
57	MG	2A	3156	1/1	0.96	0.38	61,61,61,61	0
57	MG	1W	202	1/1	0.96	0.22	48,48,48,48	0
57	MG	1A	4085	1/1	0.96	0.15	32,32,32,32	0
57	MG	1A	3753	1/1	0.96	0.21	29,29,29,29	0
57	MG	1A	3011	1/1	0.96	0.12	38,38,38,38	0
57	MG	2A	3348	1/1	0.96	0.19	58,58,58,58	0
57	MG	1A	3968	1/1	0.96	0.18	44,44,44,44	0
57	MG	1x	115	1/1	0.96	0.23	68,68,68,68	0
57	MG	1A	3755	1/1	0.96	0.14	17,17,17,17	0
57	MG	2A	3577	1/1	0.96	0.14	55,55,55,55	0
57	MG	1Y	201	1/1	0.96	0.22	47,47,47,47	0
57	MG	2a	1630	1/1	0.96	0.29	74,74,74,74	0
57	MG	2A	3165	1/1	0.96	0.13	53,53,53,53	0
57	MG	1A	3031	1/1	0.96	0.18	30,30,30,30	0
57	MG	1A	3515	1/1	0.96	0.14	46,46,46,46	0
57	MG	2a	1635	1/1	0.96	0.27	67,67,67,67	0
57	MG	1A	3868	1/1	0.96	0.23	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3585	1/1	0.96	0.13	30,30,30,30	0
57	MG	1A	3254	1/1	0.96	0.13	32,32,32,32	0
57	MG	2A	3587	1/1	0.96	0.11	46,46,46,46	0
57	MG	1A	3180	1/1	0.96	0.21	56,56,56,56	0
57	MG	1A	3587	1/1	0.96	0.11	37,37,37,37	0
57	MG	10	102	1/1	0.96	0.37	47,47,47,47	0
57	MG	2A	3173	1/1	0.96	0.21	68,68,68,68	0
57	MG	1A	3110	1/1	0.96	0.32	34,34,34,34	0
57	MG	1A	3151	1/1	0.96	0.13	31,31,31,31	0
57	MG	1A	3032	1/1	0.96	0.22	26,26,26,26	0
57	MG	1A	3980	1/1	0.96	0.15	37,37,37,37	0
57	MG	2A	3011	1/1	0.96	0.10	44,44,44,44	0
57	MG	2A	3597	1/1	0.96	0.09	35,35,35,35	0
57	MG	1A	3675	1/1	0.96	0.20	33,33,33,33	0
57	MG	1A	3521	1/1	0.96	0.19	31,31,31,31	0
57	MG	2A	3016	1/1	0.96	0.07	73,73,73,73	0
57	MG	1A	3677	1/1	0.96	0.20	25,25,25,25	0
57	MG	11	104	1/1	0.96	0.12	34,34,34,34	0
57	MG	2A	3019	1/1	0.96	0.15	30,30,30,30	0
57	MG	1A	3020	1/1	0.96	0.14	44,44,44,44	0
57	MG	12	101	1/1	0.96	0.20	39,39,39,39	0
57	MG	1A	3050	1/1	0.96	0.21	35,35,35,35	0
57	MG	1A	3772	1/1	0.96	0.21	20,20,20,20	0
57	MG	1A	3524	1/1	0.96	0.28	33,33,33,33	0
57	MG	2A	3612	1/1	0.96	0.13	41,41,41,41	0
57	MG	2A	3025	1/1	0.96	0.50	56,56,56,56	0
57	MG	1A	3186	1/1	0.96	0.23	38,38,38,38	0
57	MG	1A	3079	1/1	0.96	0.26	36,36,36,36	0
57	MG	2A	3390	1/1	0.96	0.18	45,45,45,45	0
57	MG	1A	3225	1/1	0.96	0.16	49,49,49,49	0
57	MG	1a	1733	1/1	0.96	0.30	50,50,50,50	0
57	MG	15	102	1/1	0.96	0.18	35,35,35,35	0
57	MG	15	103	1/1	0.96	0.15	29,29,29,29	0
57	MG	15	104	1/1	0.96	0.23	28,28,28,28	0
57	MG	2A	3200	1/1	0.96	0.13	52,52,52,52	0
57	MG	1a	1737	1/1	0.96	0.20	44,44,44,44	0
57	MG	1A	3991	1/1	0.96	0.20	50,50,50,50	0
57	MG	1A	3012	1/1	0.96	0.09	27,27,27,27	0
57	MG	2A	3403	1/1	0.96	0.18	60,60,60,60	0
57	MG	1B	209	1/1	0.96	0.16	36,36,36,36	0
57	MG	1A	3887	1/1	0.96	0.14	30,30,30,30	0
57	MG	17	102	1/1	0.96	0.13	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3265	1/1	0.96	0.18	62,62,62,62	0
57	MG	2A	3634	1/1	0.96	0.15	39,39,39,39	0
57	MG	1A	3418	1/1	0.96	0.13	33,33,33,33	0
57	MG	2A	3411	1/1	0.96	0.09	44,44,44,44	0
57	MG	1A	3606	1/1	0.96	0.30	51,51,51,51	0
57	MG	2A	3413	1/1	0.96	0.18	58,58,58,58	0
57	MG	1A	3607	1/1	0.96	0.21	64,64,64,64	0
57	MG	1A	3998	1/1	0.96	0.18	36,36,36,36	0
57	MG	1a	1748	1/1	0.96	0.14	60,60,60,60	0
57	MG	18	3404	1/1	0.96	0.16	42,42,42,42	0
57	MG	2A	3418	1/1	0.96	0.10	43,43,43,43	0
57	MG	2A	3419	1/1	0.96	0.15	51,51,51,51	0
57	MG	1a	1752	1/1	0.96	0.10	56,56,56,56	0
57	MG	2A	3421	1/1	0.96	0.17	40,40,40,40	0
57	MG	1A	3608	1/1	0.96	0.17	36,36,36,36	0
57	MG	1B	218	1/1	0.96	0.21	60,60,60,60	0
57	MG	2a	1700	1/1	0.96	0.16	68,68,68,68	0
57	MG	2a	1701	1/1	0.96	0.15	75,75,75,75	0
57	MG	1A	3472	1/1	0.96	0.25	31,31,31,31	0
57	MG	1A	3267	1/1	0.96	0.16	31,31,31,31	0
57	MG	2A	3221	1/1	0.96	0.19	47,47,47,47	0
57	MG	1A	3189	1/1	0.96	0.12	30,30,30,30	0
57	MG	2A	3655	1/1	0.96	0.28	57,57,57,57	0
57	MG	1A	3162	1/1	0.96	0.35	33,33,33,33	0
57	MG	1A	3231	1/1	0.96	0.19	48,48,48,48	0
57	MG	1A	3063	1/1	0.96	0.20	26,26,26,26	0
57	MG	1A	3424	1/1	0.96	0.22	53,53,53,53	0
57	MG	1A	3797	1/1	0.96	0.11	48,48,48,48	0
57	MG	2A	3228	1/1	0.96	0.33	59,59,59,59	0
57	MG	1a	1608	1/1	0.96	0.20	50,50,50,50	0
57	MG	1A	4008	1/1	0.96	0.20	28,28,28,28	0
57	MG	2A	3665	1/1	0.96	0.17	45,45,45,45	0
57	MG	1a	1611	1/1	0.96	0.17	28,28,28,28	0
57	MG	2A	3441	1/1	0.96	0.25	59,59,59,59	0
57	MG	1A	4009	1/1	0.96	0.15	16,16,16,16	0
57	MG	1A	4010	1/1	0.96	0.20	27,27,27,27	0
57	MG	1A	4011	1/1	0.96	0.20	19,19,19,19	0
57	MG	2A	3672	1/1	0.96	0.12	40,40,40,40	0
57	MG	1A	3272	1/1	0.96	0.16	38,38,38,38	0
57	MG	1a	1775	1/1	0.96	0.11	51,51,51,51	0
57	MG	2a	1725	1/1	0.96	0.29	66,66,66,66	0
57	MG	1A	3801	1/1	0.96	0.27	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3448	1/1	0.96	0.14	42,42,42,42	0
57	MG	2A	3678	1/1	0.96	0.14	50,50,50,50	0
57	MG	1A	3802	1/1	0.96	0.12	58,58,58,58	0
57	MG	2A	3239	1/1	0.96	0.27	55,55,55,55	0
57	MG	2A	3240	1/1	0.96	0.20	57,57,57,57	0
57	MG	1a	1620	1/1	0.96	0.12	54,54,54,54	0
57	MG	1A	3084	1/1	0.96	0.26	27,27,27,27	0
57	MG	2a	1734	1/1	0.96	0.28	55,55,55,55	0
57	MG	2A	3072	1/1	0.96	0.22	48,48,48,48	0
57	MG	2A	3456	1/1	0.96	0.18	55,55,55,55	0
57	MG	1A	3040	1/1	0.96	0.12	39,39,39,39	0
57	MG	2A	3458	1/1	0.96	0.10	55,55,55,55	0
57	MG	1A	4018	1/1	0.96	0.06	33,33,33,33	0
57	MG	1A	3166	1/1	0.96	0.28	32,32,32,32	0
57	MG	2A	3691	1/1	0.96	0.15	30,30,30,30	0
57	MG	1A	3910	1/1	0.96	0.19	52,52,52,52	0
57	MG	1A	3911	1/1	0.96	0.14	46,46,46,46	0
57	MG	2a	1744	1/1	0.96	0.24	55,55,55,55	0
57	MG	2A	3463	1/1	0.96	0.23	63,63,63,63	0
57	MG	1A	3912	1/1	0.96	0.13	30,30,30,30	0
57	MG	1A	3806	1/1	0.96	0.23	21,21,21,21	0
57	MG	1E	302	1/1	0.96	0.31	32,32,32,32	0
57	MG	1A	3236	1/1	0.96	0.24	27,27,27,27	0
57	MG	2A	3699	1/1	0.96	0.20	48,48,48,48	0
57	MG	1A	3712	1/1	0.96	0.18	27,27,27,27	0
57	MG	1A	4029	1/1	0.96	0.31	77,77,77,77	0
57	MG	2A	3084	1/1	0.96	0.21	50,50,50,50	0
57	MG	1A	3916	1/1	0.96	0.15	35,35,35,35	0
57	MG	1E	309	1/1	0.96	0.30	53,53,53,53	0
57	MG	1A	3623	1/1	0.96	0.11	42,42,42,42	0
57	MG	1A	3624	1/1	0.96	0.15	21,21,21,21	0
57	MG	2A	3709	1/1	0.96	0.13	64,64,64,64	0
57	MG	2A	3479	1/1	0.96	0.07	56,56,56,56	0
57	MG	2A	3480	1/1	0.96	0.13	50,50,50,50	0
57	MG	1A	3488	1/1	0.96	0.25	38,38,38,38	0
57	MG	2A	3714	1/1	0.96	0.06	73,73,73,73	0
57	MG	1A	3237	1/1	0.96	0.23	30,30,30,30	0
57	MG	1a	1798	1/1	0.96	0.07	64,64,64,64	0
57	MG	1A	3629	1/1	0.96	0.15	50,50,50,50	0
57	MG	2A	3718	1/1	0.96	0.18	57,57,57,57	0
57	MG	2A	3267	1/1	0.96	0.18	38,38,38,38	0
57	MG	1F	301	1/1	0.96	0.35	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3487	1/1	0.96	0.11	44,44,44,44	0
57	MG	2A	3488	1/1	0.96	0.12	34,34,34,34	0
57	MG	2A	3724	1/1	0.96	0.18	44,44,44,44	0
57	MG	2A	3727	1/1	0.96	0.09	58,58,58,58	0
57	MG	2a	1774	1/1	0.96	0.10	61,61,61,61	0
57	MG	1F	302	1/1	0.96	0.17	31,31,31,31	0
57	MG	1A	3432	1/1	0.96	0.12	39,39,39,39	0
57	MG	2A	3271	1/1	0.96	0.28	62,62,62,62	0
57	MG	1F	305	1/1	0.96	0.23	34,34,34,34	0
57	MG	2B	202	1/1	0.96	0.34	60,60,60,60	0
57	MG	1A	3382	1/1	0.96	0.16	34,34,34,34	0
57	MG	2A	3494	1/1	0.96	0.10	39,39,39,39	0
57	MG	2a	1783	1/1	0.96	0.23	73,73,73,73	0
57	MG	2A	3274	1/1	0.96	0.45	48,48,48,48	0
57	MG	1A	3280	1/1	0.96	0.38	38,38,38,38	0
57	MG	1F	310	1/1	0.96	0.18	30,30,30,30	0
57	MG	1A	4040	1/1	0.96	0.18	24,24,24,24	0
57	MG	1A	3201	1/1	0.96	0.14	32,32,32,32	0
57	MG	1A	3637	1/1	0.96	0.09	42,42,42,42	0
57	MG	1A	3725	1/1	0.96	0.13	16,16,16,16	0
57	MG	1A	3824	1/1	0.96	0.18	55,55,55,55	0
57	MG	1A	3240	1/1	0.96	0.17	31,31,31,31	0
57	MG	1G	205	1/1	0.96	0.10	53,53,53,53	0
57	MG	2A	3507	1/1	0.96	0.11	65,65,65,65	0
57	MG	1A	3826	1/1	0.96	0.12	31,31,31,31	0
57	MG	2t	201	1/1	0.96	0.13	45,45,45,45	0
57	MG	1A	3241	1/1	0.96	0.25	29,29,29,29	0
57	MG	2A	3290	1/1	0.96	0.23	45,45,45,45	0
57	MG	1A	3640	1/1	0.96	0.10	19,19,19,19	0
57	MG	1N	203	1/1	0.96	0.20	41,41,41,41	0
57	MG	1A	3140	1/1	0.96	0.17	27,27,27,27	0
57	MG	2D	306	1/1	0.96	0.72	42,42,42,42	0
57	MG	2E	301	1/1	0.96	0.25	59,59,59,59	0
57	MG	1a	1822	1/1	0.96	0.10	50,50,50,50	0
57	MG	1A	3203	1/1	0.96	0.19	22,22,22,22	0
58	6IF	2A	3731	32/32	0.96	0.24	28,36,41,45	0
57	MG	1A	3834	1/1	0.96	0.14	40,40,40,40	0
59	ZN	2Y	202	1/1	0.96	0.12	95,95,95,95	0
57	MG	1A	3732	1/1	0.96	0.19	25,25,25,25	0
57	MG	2E	306	1/1	0.96	0.22	57,57,57,57	0
57	MG	2E	307	1/1	0.96	0.15	35,35,35,35	0
57	MG	2A	3298	1/1	0.96	0.33	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1P	202	1/1	0.97	0.14	25,25,25,25	0
57	MG	1A	3302	1/1	0.97	0.34	54,54,54,54	0
57	MG	1A	3160	1/1	0.97	0.20	27,27,27,27	0
57	MG	2A	3609	1/1	0.97	0.16	53,53,53,53	0
57	MG	1A	3430	1/1	0.97	0.31	36,36,36,36	0
57	MG	1Q	202	1/1	0.97	0.17	36,36,36,36	0
57	MG	1A	3266	1/1	0.97	0.23	41,41,41,41	0
57	MG	1A	3113	1/1	0.97	0.11	33,33,33,33	0
57	MG	1A	4084	1/1	0.97	0.10	32,32,32,32	0
57	MG	1A	3541	1/1	0.97	0.22	45,45,45,45	0
57	MG	1A	3695	1/1	0.97	0.17	23,23,23,23	0
57	MG	1A	4087	1/1	0.97	0.29	55,55,55,55	0
57	MG	2A	3245	1/1	0.97	0.17	49,49,49,49	0
57	MG	1a	1806	1/1	0.97	0.10	68,68,68,68	0
57	MG	1A	3485	1/1	0.97	0.16	41,41,41,41	0
57	MG	2A	3090	1/1	0.97	0.17	51,51,51,51	0
57	MG	2A	3250	1/1	0.97	0.06	59,59,59,59	0
57	MG	2a	1634	1/1	0.97	0.12	72,72,72,72	0
57	MG	1A	3038	1/1	0.97	0.30	30,30,30,30	0
57	MG	1A	3698	1/1	0.97	0.16	22,22,22,22	0
57	MG	1A	4091	1/1	0.97	0.14	57,57,57,57	0
57	MG	1A	3127	1/1	0.97	0.22	40,40,40,40	0
57	MG	1A	3617	1/1	0.97	0.16	22,22,22,22	0
57	MG	2A	3631	1/1	0.97	0.16	56,56,56,56	0
57	MG	1A	3782	1/1	0.97	0.11	47,47,47,47	0
57	MG	1A	3309	1/1	0.97	0.18	37,37,37,37	0
57	MG	1A	3883	1/1	0.97	0.16	34,34,34,34	0
57	MG	1U	203	1/1	0.97	0.19	28,28,28,28	0
57	MG	2a	1645	1/1	0.97	0.08	54,54,54,54	0
57	MG	1U	204	1/1	0.97	0.24	32,32,32,32	0
57	MG	2a	1647	1/1	0.97	0.36	76,76,76,76	0
57	MG	1U	205	1/1	0.97	0.20	30,30,30,30	0
57	MG	1U	207	1/1	0.97	0.28	32,32,32,32	0
57	MG	1a	1820	1/1	0.97	0.24	51,51,51,51	0
57	MG	1A	3619	1/1	0.97	0.17	27,27,27,27	0
57	MG	1a	1674	1/1	0.97	0.12	66,66,66,66	0
57	MG	1A	3391	1/1	0.97	0.26	51,51,51,51	0
57	MG	1A	3788	1/1	0.97	0.10	21,21,21,21	0
57	MG	1A	3211	1/1	0.97	0.26	32,32,32,32	0
57	MG	1A	3791	1/1	0.97	0.09	48,48,48,48	0
57	MG	1A	4102	1/1	0.97	0.16	46,46,46,46	0
57	MG	1A	3082	1/1	0.97	0.28	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3351	1/1	0.97	0.22	40,40,40,40	0
57	MG	1A	3440	1/1	0.97	0.24	37,37,37,37	0
57	MG	1A	3709	1/1	0.97	0.24	23,23,23,23	0
57	MG	2a	1662	1/1	0.97	0.12	55,55,55,55	0
57	MG	1X	101	1/1	0.97	0.40	38,38,38,38	0
57	MG	1A	3213	1/1	0.97	0.13	38,38,38,38	0
57	MG	1B	201	1/1	0.97	0.23	51,51,51,51	0
57	MG	1A	3626	1/1	0.97	0.19	10,10,10,10	0
57	MG	1A	3800	1/1	0.97	0.22	20,20,20,20	0
57	MG	1A	3314	1/1	0.97	0.18	59,59,59,59	0
57	MG	2A	3122	1/1	0.97	0.33	48,48,48,48	0
57	MG	2A	3283	1/1	0.97	0.30	43,43,43,43	0
57	MG	2A	3123	1/1	0.97	0.10	37,37,37,37	0
57	MG	2A	3285	1/1	0.97	0.28	44,44,44,44	0
57	MG	1A	3046	1/1	0.97	0.21	30,30,30,30	0
57	MG	2A	3473	1/1	0.97	0.16	68,68,68,68	0
57	MG	1A	3215	1/1	0.97	0.26	38,38,38,38	0
57	MG	1A	3633	1/1	0.97	0.21	42,42,42,42	0
57	MG	2a	1677	1/1	0.97	0.23	71,71,71,71	0
57	MG	1A	3357	1/1	0.97	0.25	48,48,48,48	0
57	MG	1A	3499	1/1	0.97	0.12	38,38,38,38	0
57	MG	1A	3807	1/1	0.97	0.22	26,26,26,26	0
57	MG	1A	3446	1/1	0.97	0.19	44,44,44,44	0
57	MG	1A	3146	1/1	0.97	0.18	29,29,29,29	0
57	MG	1a	1699	1/1	0.97	0.24	44,44,44,44	0
57	MG	1A	3721	1/1	0.97	0.14	45,45,45,45	0
57	MG	1A	3907	1/1	0.97	0.13	43,43,43,43	0
57	MG	1A	3047	1/1	0.97	0.18	28,28,28,28	0
57	MG	1A	3503	1/1	0.97	0.26	45,45,45,45	0
57	MG	1A	3085	1/1	0.97	0.27	32,32,32,32	0
57	MG	1A	3815	1/1	0.97	0.15	24,24,24,24	0
57	MG	1B	220	1/1	0.97	0.20	50,50,50,50	0
57	MG	1A	3450	1/1	0.97	0.15	32,32,32,32	0
57	MG	1B	222	1/1	0.97	0.12	51,51,51,51	0
57	MG	2A	3144	1/1	0.97	0.04	55,55,55,55	0
57	MG	1A	3404	1/1	0.97	0.28	29,29,29,29	0
57	MG	1x	109	1/1	0.97	0.10	59,59,59,59	0
57	MG	1A	3727	1/1	0.97	0.10	27,27,27,27	0
57	MG	1A	3279	1/1	0.97	0.17	30,30,30,30	0
57	MG	1A	3570	1/1	0.97	0.20	41,41,41,41	0
57	MG	1a	1714	1/1	0.97	0.12	46,46,46,46	0
57	MG	15	101	1/1	0.97	0.21	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3132	1/1	0.97	0.18	40,40,40,40	0
57	MG	2A	3501	1/1	0.97	0.15	54,54,54,54	0
57	MG	2A	3502	1/1	0.97	0.15	37,37,37,37	0
57	MG	1A	3283	1/1	0.97	0.61	35,35,35,35	0
57	MG	1A	3323	1/1	0.97	0.18	61,61,61,61	0
57	MG	2A	3317	1/1	0.97	0.15	53,53,53,53	0
57	MG	1A	4021	1/1	0.97	0.07	36,36,36,36	0
57	MG	1A	4022	1/1	0.97	0.16	30,30,30,30	0
57	MG	1A	3409	1/1	0.97	0.22	42,42,42,42	0
57	MG	2A	3704	1/1	0.97	0.06	53,53,53,53	0
57	MG	15	109	1/1	0.97	0.13	57,57,57,57	0
57	MG	2a	1713	1/1	0.97	0.13	62,62,62,62	0
57	MG	2A	3322	1/1	0.97	0.25	48,48,48,48	0
57	MG	1A	4024	1/1	0.97	0.20	33,33,33,33	0
57	MG	17	101	1/1	0.97	0.14	29,29,29,29	0
57	MG	1A	3066	1/1	0.97	0.15	25,25,25,25	0
57	MG	2A	3327	1/1	0.97	0.21	41,41,41,41	0
57	MG	2A	3006	1/1	0.97	0.27	46,46,46,46	0
57	MG	1A	3925	1/1	0.97	0.19	35,35,35,35	0
57	MG	17	104	1/1	0.97	0.15	31,31,31,31	0
57	MG	1D	301	1/1	0.97	0.21	28,28,28,28	0
57	MG	1A	3576	1/1	0.97	0.23	24,24,24,24	0
57	MG	1a	1732	1/1	0.97	0.13	42,42,42,42	0
57	MG	2A	3335	1/1	0.97	0.07	62,62,62,62	0
57	MG	1A	3927	1/1	0.97	0.23	33,33,33,33	0
57	MG	18	3402	1/1	0.97	0.16	37,37,37,37	0
57	MG	2A	3721	1/1	0.97	0.14	45,45,45,45	0
57	MG	1A	3828	1/1	0.97	0.41	34,34,34,34	0
57	MG	1A	3578	1/1	0.97	0.18	24,24,24,24	0
57	MG	2A	3526	1/1	0.97	0.10	49,49,49,49	0
57	MG	2A	3527	1/1	0.97	0.19	51,51,51,51	0
57	MG	1A	3654	1/1	0.97	0.32	24,24,24,24	0
57	MG	1D	310	1/1	0.97	0.20	30,30,30,30	0
57	MG	1A	4032	1/1	0.97	0.11	50,50,50,50	0
57	MG	1A	3832	1/1	0.97	0.13	27,27,27,27	0
57	MG	1A	3286	1/1	0.97	0.23	35,35,35,35	0
57	MG	1A	3109	1/1	0.97	0.11	38,38,38,38	0
57	MG	2A	3347	1/1	0.97	0.29	39,39,39,39	0
57	MG	1A	3222	1/1	0.97	0.22	28,28,28,28	0
57	MG	1A	3836	1/1	0.97	0.11	34,34,34,34	0
57	MG	1A	3195	1/1	0.97	0.29	52,52,52,52	0
57	MG	1A	3659	1/1	0.97	0.14	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3839	1/1	0.97	0.16	36,36,36,36	0
57	MG	2B	210	1/1	0.97	0.32	61,61,61,61	0
57	MG	2A	3541	1/1	0.97	0.10	43,43,43,43	0
57	MG	1a	1609	1/1	0.97	0.18	48,48,48,48	0
57	MG	2a	1748	1/1	0.97	0.31	62,62,62,62	0
57	MG	1a	1749	1/1	0.97	0.16	59,59,59,59	0
57	MG	1a	1750	1/1	0.97	0.18	44,44,44,44	0
57	MG	1A	3196	1/1	0.97	0.20	41,41,41,41	0
57	MG	2A	3357	1/1	0.97	0.14	64,64,64,64	0
57	MG	1A	3175	1/1	0.97	0.16	26,26,26,26	0
57	MG	1A	3199	1/1	0.97	0.23	24,24,24,24	0
57	MG	2A	3035	1/1	0.97	0.18	31,31,31,31	0
57	MG	1a	1613	1/1	0.97	0.06	65,65,65,65	0
57	MG	1a	1614	1/1	0.97	0.22	54,54,54,54	0
57	MG	1A	3200	1/1	0.97	0.22	31,31,31,31	0
57	MG	1A	3943	1/1	0.97	0.10	51,51,51,51	0
57	MG	1E	316	1/1	0.97	0.08	44,44,44,44	0
57	MG	1A	3944	1/1	0.97	0.14	12,12,12,12	0
57	MG	2A	3369	1/1	0.97	0.20	61,61,61,61	0
57	MG	2A	3559	1/1	0.97	0.08	61,61,61,61	0
57	MG	1A	3076	1/1	0.97	0.11	33,33,33,33	0
57	MG	1a	1761	1/1	0.97	0.14	42,42,42,42	0
57	MG	1F	303	1/1	0.97	0.19	31,31,31,31	0
57	MG	2A	3046	1/1	0.97	0.35	46,46,46,46	0
57	MG	1a	1621	1/1	0.97	0.17	45,45,45,45	0
57	MG	2F	304	1/1	0.97	0.49	47,47,47,47	0
57	MG	1A	3468	1/1	0.97	0.19	50,50,50,50	0
57	MG	2A	3377	1/1	0.97	0.33	56,56,56,56	0
57	MG	2A	3568	1/1	0.97	0.15	58,58,58,58	0
57	MG	1A	3947	1/1	0.97	0.15	29,29,29,29	0
57	MG	1A	3155	1/1	0.97	0.15	40,40,40,40	0
57	MG	1A	3949	1/1	0.97	0.18	30,30,30,30	0
57	MG	1a	1768	1/1	0.97	0.15	38,38,38,38	0
57	MG	2A	3208	1/1	0.97	0.32	58,58,58,58	0
57	MG	2A	3574	1/1	0.97	0.35	77,77,77,77	0
57	MG	2T	203	1/1	0.97	0.13	48,48,48,48	0
57	MG	1A	3669	1/1	0.97	0.19	31,31,31,31	0
57	MG	2A	3385	1/1	0.97	0.24	60,60,60,60	0
57	MG	1A	4055	1/1	0.97	0.09	46,46,46,46	0
57	MG	1A	3056	1/1	0.97	0.18	28,28,28,28	0
57	MG	1a	1773	1/1	0.97	0.09	57,57,57,57	0
57	MG	2a	1786	1/1	0.97	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
57	MG	2A	3580	1/1	0.97	0.10	49,49,49,49	0
57	MG	1a	1774	1/1	0.97	0.08	50,50,50,50	0
57	MG	1A	3204	1/1	0.97	0.12	34,34,34,34	0
57	MG	2A	3393	1/1	0.97	0.12	48,48,48,48	0
57	MG	2A	3584	1/1	0.97	0.15	32,32,32,32	0
57	MG	2l	202	1/1	0.97	0.22	65,65,65,65	0
57	MG	1A	3851	1/1	0.97	0.21	34,34,34,34	0
57	MG	1A	3009	1/1	0.97	0.12	22,22,22,22	0
57	MG	1A	3528	1/1	0.97	0.25	47,47,47,47	0
57	MG	1A	3473	1/1	0.97	0.11	35,35,35,35	0
57	MG	1A	4062	1/1	0.97	0.19	40,40,40,40	0
57	MG	1A	3598	1/1	0.97	0.20	28,28,28,28	0
57	MG	1A	3380	1/1	0.97	0.42	40,40,40,40	0
57	MG	2A	3401	1/1	0.97	0.12	44,44,44,44	0
57	MG	1a	1783	1/1	0.97	0.08	71,71,71,71	0
57	MG	1A	3475	1/1	0.97	0.11	47,47,47,47	0
57	MG	1A	3602	1/1	0.97	0.24	37,37,37,37	0
57	MG	2A	3406	1/1	0.97	0.18	66,66,66,66	0
57	MG	2x	105	1/1	0.97	0.13	54,54,54,54	0
57	MG	1A	3859	1/1	0.97	0.15	43,43,43,43	0
57	MG	1A	3381	1/1	0.97	0.18	49,49,49,49	0
57	MG	1A	3862	1/1	0.97	0.17	56,56,56,56	0
58	6IF	1A	4109	32/32	0.97	0.21	18,25,31,31	0
57	MG	1A	3764	1/1	0.97	0.11	25,25,25,25	0
57	MG	1A	3477	1/1	0.97	0.20	51,51,51,51	0
57	MG	1A	3684	1/1	0.97	0.16	20,20,20,20	0
57	MG	1A	3300	1/1	0.97	0.29	45,45,45,45	0
57	MG	2A	3604	1/1	0.97	0.13	53,53,53,53	0
59	ZN	29	501	1/1	0.97	0.10	66,66,66,66	0
57	MG	2a	1613	1/1	0.97	0.09	63,63,63,63	0
57	MG	1A	3124	1/1	0.97	0.20	32,32,32,32	0
57	MG	1A	3033	1/1	0.98	0.17	27,27,27,27	0
57	MG	2a	1682	1/1	0.98	0.17	66,66,66,66	0
57	MG	2A	3367	1/1	0.98	0.29	39,39,39,39	0
57	MG	1a	1730	1/1	0.98	0.19	43,43,43,43	0
57	MG	1A	3287	1/1	0.98	0.15	39,39,39,39	0
57	MG	2A	3611	1/1	0.98	0.18	55,55,55,55	0
57	MG	1A	3350	1/1	0.98	0.47	37,37,37,37	0
57	MG	1A	3013	1/1	0.98	0.27	30,30,30,30	0
57	MG	1X	104	1/1	0.98	0.25	33,33,33,33	0
57	MG	1X	105	1/1	0.98	0.09	42,42,42,42	0
57	MG	1A	3192	1/1	0.98	0.27	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3618	1/1	0.98	0.09	54,54,54,54	0
57	MG	1A	4083	1/1	0.98	0.12	43,43,43,43	0
57	MG	2A	3376	1/1	0.98	0.24	47,47,47,47	0
57	MG	2D	305	1/1	0.98	0.13	31,31,31,31	0
57	MG	1A	3108	1/1	0.98	0.23	26,26,26,26	0
57	MG	1A	3154	1/1	0.98	0.20	35,35,35,35	0
57	MG	1A	3239	1/1	0.98	0.27	30,30,30,30	0
57	MG	1E	311	1/1	0.98	0.18	38,38,38,38	0
57	MG	2A	3381	1/1	0.98	0.15	60,60,60,60	0
57	MG	1A	3453	1/1	0.98	0.18	38,38,38,38	0
57	MG	1A	3138	1/1	0.98	0.29	33,33,33,33	0
57	MG	1A	4016	1/1	0.98	0.14	21,21,21,21	0
57	MG	1n	101	1/1	0.98	0.29	53,53,53,53	0
57	MG	10	104	1/1	0.98	0.34	34,34,34,34	0
57	MG	1A	3645	1/1	0.98	0.15	24,24,24,24	0
57	MG	2A	3277	1/1	0.98	0.17	61,61,61,61	0
57	MG	2A	3389	1/1	0.98	0.10	24,24,24,24	0
57	MG	1A	3156	1/1	0.98	0.34	31,31,31,31	0
57	MG	2A	3391	1/1	0.98	0.14	43,43,43,43	0
57	MG	1A	3600	1/1	0.98	0.15	35,35,35,35	0
57	MG	1A	3242	1/1	0.98	0.43	33,33,33,33	0
57	MG	1A	3197	1/1	0.98	0.15	32,32,32,32	0
57	MG	1A	3069	1/1	0.98	0.22	21,21,21,21	0
57	MG	1A	3705	1/1	0.98	0.13	38,38,38,38	0
57	MG	1F	307	1/1	0.98	0.22	34,34,34,34	0
57	MG	1A	3178	1/1	0.98	0.19	31,31,31,31	0
57	MG	1A	3605	1/1	0.98	0.11	29,29,29,29	0
57	MG	1A	3766	1/1	0.98	0.20	59,59,59,59	0
57	MG	1A	3526	1/1	0.98	0.15	25,25,25,25	0
57	MG	2A	3647	1/1	0.98	0.06	53,53,53,53	0
57	MG	1A	3081	1/1	0.98	0.32	41,41,41,41	0
57	MG	1A	3831	1/1	0.98	0.14	24,24,24,24	0
57	MG	2I	101	1/1	0.98	0.50	52,52,52,52	0
57	MG	1A	3563	1/1	0.98	0.19	34,34,34,34	0
57	MG	1A	4104	1/1	0.98	0.23	49,49,49,49	0
57	MG	1A	3036	1/1	0.98	0.17	23,23,23,23	0
57	MG	25	102	1/1	0.98	0.48	45,45,45,45	0
57	MG	1A	3897	1/1	0.98	0.14	41,41,41,41	0
57	MG	2A	3528	1/1	0.98	0.15	63,63,63,63	0
57	MG	1A	3565	1/1	0.98	0.21	49,49,49,49	0
57	MG	1A	3566	1/1	0.98	0.16	32,32,32,32	0
57	MG	15	106	1/1	0.98	0.14	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3071	1/1	0.98	0.18	16,16,16,16	0
57	MG	1A	3037	1/1	0.98	0.21	31,31,31,31	0
57	MG	1A	3662	1/1	0.98	0.10	36,36,36,36	0
57	MG	2A	3661	1/1	0.98	0.10	62,62,62,62	0
57	MG	1a	1770	1/1	0.98	0.21	60,60,60,60	0
57	MG	1A	3569	1/1	0.98	0.23	44,44,44,44	0
57	MG	1N	206	1/1	0.98	0.25	30,30,30,30	0
57	MG	1A	3030	1/1	0.98	0.17	28,28,28,28	0
57	MG	1A	3841	1/1	0.98	0.22	40,40,40,40	0
57	MG	1A	4041	1/1	0.98	0.11	45,45,45,45	0
57	MG	1A	3665	1/1	0.98	0.20	36,36,36,36	0
57	MG	2A	3669	1/1	0.98	0.14	41,41,41,41	0
57	MG	1A	3022	1/1	0.98	0.14	36,36,36,36	0
57	MG	2A	3423	1/1	0.98	0.19	26,26,26,26	0
57	MG	1A	3001	1/1	0.98	0.21	34,34,34,34	0
57	MG	1a	1685	1/1	0.98	0.10	43,43,43,43	0
57	MG	1A	3229	1/1	0.98	0.32	31,31,31,31	0
57	MG	2A	3427	1/1	0.98	0.12	37,37,37,37	0
57	MG	2A	3676	1/1	0.98	0.12	36,36,36,36	0
57	MG	1A	3403	1/1	0.98	0.21	27,27,27,27	0
57	MG	1A	3783	1/1	0.98	0.15	17,17,17,17	0
57	MG	2A	3315	1/1	0.98	0.22	59,59,59,59	0
57	MG	1P	204	1/1	0.98	0.31	31,31,31,31	0
57	MG	2A	3432	1/1	0.98	0.17	68,68,68,68	0
57	MG	2A	3012	1/1	0.98	0.10	42,42,42,42	0
57	MG	2A	3013	1/1	0.98	0.17	53,53,53,53	0
57	MG	2a	1624	1/1	0.98	0.11	59,59,59,59	0
57	MG	1A	3278	1/1	0.98	0.17	25,25,25,25	0
57	MG	1A	3088	1/1	0.98	0.39	34,34,34,34	0
57	MG	2A	3558	1/1	0.98	0.13	62,62,62,62	0
57	MG	2a	1628	1/1	0.98	0.11	83,83,83,83	0
57	MG	1Q	201	1/1	0.98	0.21	29,29,29,29	0
57	MG	1A	3577	1/1	0.98	0.24	21,21,21,21	0
57	MG	2A	3323	1/1	0.98	0.39	52,52,52,52	0
57	MG	2A	3219	1/1	0.98	0.22	50,50,50,50	0
57	MG	1A	4051	1/1	0.98	0.24	28,28,28,28	0
57	MG	1A	3041	1/1	0.98	0.19	27,27,27,27	0
57	MG	1A	3311	1/1	0.98	0.29	50,50,50,50	0
57	MG	2A	3566	1/1	0.98	0.19	35,35,35,35	0
57	MG	1A	3918	1/1	0.98	0.14	36,36,36,36	0
57	MG	1A	3790	1/1	0.98	0.10	29,29,29,29	0
57	MG	1A	3281	1/1	0.98	0.22	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1a	1700	1/1	0.98	0.25	45,45,45,45	0
57	MG	2A	3700	1/1	0.98	0.06	58,58,58,58	0
57	MG	1A	3282	1/1	0.98	0.45	35,35,35,35	0
57	MG	1A	3922	1/1	0.98	0.15	20,20,20,20	0
57	MG	1A	3168	1/1	0.98	0.32	38,38,38,38	0
57	MG	1A	3077	1/1	0.98	0.24	24,24,24,24	0
57	MG	2A	3453	1/1	0.98	0.14	24,24,24,24	0
57	MG	1A	3795	1/1	0.98	0.20	43,43,43,43	0
57	MG	1A	3285	1/1	0.98	0.18	44,44,44,44	0
57	MG	1A	3860	1/1	0.98	0.21	15,15,15,15	0
57	MG	2A	3131	1/1	0.98	0.34	38,38,38,38	0
57	MG	1A	3631	1/1	0.98	0.23	27,27,27,27	0
57	MG	1A	3798	1/1	0.98	0.07	36,36,36,36	0
57	MG	1A	3681	1/1	0.98	0.14	41,41,41,41	0
57	MG	2A	3713	1/1	0.98	0.16	44,44,44,44	0
57	MG	1A	3682	1/1	0.98	0.15	19,19,19,19	0
57	MG	2A	3345	1/1	0.98	0.18	54,54,54,54	0
57	MG	1A	3865	1/1	0.98	0.26	17,17,17,17	0
57	MG	2A	3464	1/1	0.98	0.14	38,38,38,38	0
57	MG	1A	3683	1/1	0.98	0.23	24,24,24,24	0
57	MG	1A	3632	1/1	0.98	0.19	24,24,24,24	0
57	MG	1A	3585	1/1	0.98	0.32	33,33,33,33	0
57	MG	1V	201	1/1	0.98	0.25	24,24,24,24	0
57	MG	1D	304	1/1	0.98	0.11	21,21,21,21	0
57	MG	1V	203	1/1	0.98	0.23	30,30,30,30	0
57	MG	2A	3471	1/1	0.98	0.12	57,57,57,57	0
57	MG	2A	3725	1/1	0.98	0.14	62,62,62,62	0
57	MG	2A	3726	1/1	0.98	0.13	53,53,53,53	0
57	MG	1A	4072	1/1	0.98	0.20	15,15,15,15	0
57	MG	1D	307	1/1	0.98	0.23	36,36,36,36	0
57	MG	2A	3045	1/1	0.98	0.16	26,26,26,26	0
57	MG	2A	3249	1/1	0.98	0.11	49,49,49,49	0
57	MG	1V	206	1/1	0.98	0.23	48,48,48,48	0
57	MG	1A	3686	1/1	0.98	0.12	26,26,26,26	0
59	ZN	1Y	205	1/1	0.98	0.20	57,57,57,57	0
57	MG	1A	4075	1/1	0.98	0.19	23,23,23,23	0
59	ZN	19	102	1/1	0.98	0.30	67,67,67,67	0
57	MG	1a	1632	1/1	0.98	0.20	59,59,59,59	0
57	MG	1W	203	1/1	0.98	0.27	35,35,35,35	0
59	ZN	25	104	1/1	0.98	0.20	57,57,57,57	0
57	MG	1A	3545	1/1	0.98	0.22	59,59,59,59	0
57	MG	1a	1727	1/1	0.98	0.24	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3364	1/1	0.98	0.12	47,47,47,47	0
60	SF4	2d	302	8/8	0.98	0.12	62,75,82,85	0
57	MG	1A	3688	1/1	0.98	0.13	27,27,27,27	0
57	MG	1Y	204	1/1	0.99	0.24	36,36,36,36	0
57	MG	1A	3328	1/1	0.99	0.29	41,41,41,41	0
57	MG	2A	3289	1/1	0.99	0.27	43,43,43,43	0
57	MG	1A	3014	1/1	0.99	0.18	23,23,23,23	0
57	MG	1F	306	1/1	0.99	0.25	28,28,28,28	0
57	MG	1A	3021	1/1	0.99	0.20	22,22,22,22	0
57	MG	2A	3436	1/1	0.99	0.15	36,36,36,36	0
57	MG	1A	3068	1/1	0.99	0.21	26,26,26,26	0
57	MG	1B	235	1/1	0.99	0.09	35,35,35,35	0
57	MG	1A	3008	1/1	0.99	0.18	24,24,24,24	0
57	MG	1A	3023	1/1	0.99	0.15	18,18,18,18	0
57	MG	2a	1777	1/1	0.99	0.24	73,73,73,73	0
57	MG	1A	3134	1/1	0.99	0.18	25,25,25,25	0
57	MG	2A	3115	1/1	0.99	0.17	35,35,35,35	0
57	MG	2A	3646	1/1	0.99	0.09	48,48,48,48	0
57	MG	1A	3035	1/1	0.99	0.11	32,32,32,32	0
57	MG	10	108	1/1	0.99	0.15	46,46,46,46	0
57	MG	1A	3228	1/1	0.99	0.31	24,24,24,24	0
57	MG	2A	3546	1/1	0.99	0.18	41,41,41,41	0
57	MG	1A	3784	1/1	0.99	0.19	22,22,22,22	0
57	MG	1D	306	1/1	0.99	0.22	26,26,26,26	0
57	MG	1A	3354	1/1	0.99	0.15	35,35,35,35	0
57	MG	1A	3759	1/1	0.99	0.14	33,33,33,33	0
57	MG	1U	206	1/1	0.99	0.33	33,33,33,33	0
57	MG	2F	303	1/1	0.99	0.25	53,53,53,53	0
57	MG	1A	3814	1/1	0.99	0.13	22,22,22,22	0
57	MG	1A	3304	1/1	0.99	0.22	23,23,23,23	0
57	MG	1A	3096	1/1	0.99	0.24	22,22,22,22	0
57	MG	2A	3405	1/1	0.99	0.16	24,24,24,24	0
57	MG	1A	3106	1/1	0.99	0.22	31,31,31,31	0
57	MG	1A	3818	1/1	0.99	0.31	26,26,26,26	0
57	MG	1B	215	1/1	0.99	0.17	35,35,35,35	0
57	MG	1A	3627	1/1	0.99	0.22	37,37,37,37	0
57	MG	1A	3738	1/1	0.99	0.10	52,52,52,52	0
57	MG	1E	305	1/1	0.99	0.21	28,28,28,28	0
57	MG	1A	3908	1/1	0.99	0.15	28,28,28,28	0
57	MG	2A	3614	1/1	0.99	0.34	45,45,45,45	0
57	MG	1A	3586	1/1	0.99	0.10	32,32,32,32	0
57	MG	2A	3135	1/1	0.99	0.19	54,54,54,54	0

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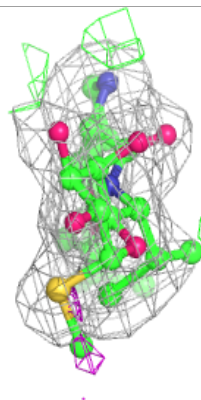
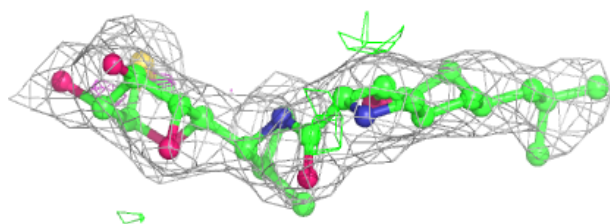
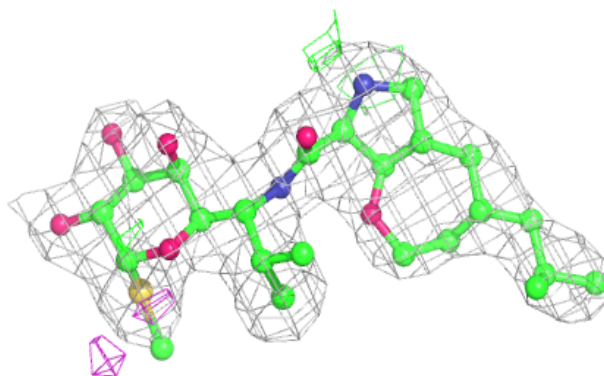
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1E	308	1/1	0.99	0.10	30,30,30,30	0
57	MG	1A	3740	1/1	0.99	0.16	44,44,44,44	0
57	MG	1A	3174	1/1	0.99	0.21	25,25,25,25	0
57	MG	2A	3183	1/1	0.99	0.06	58,58,58,58	0
57	MG	1a	1668	1/1	0.99	0.12	57,57,57,57	0
57	MG	1A	3717	1/1	0.99	0.20	27,27,27,27	0
57	MG	2A	3186	1/1	0.99	0.27	40,40,40,40	0
57	MG	1A	3651	1/1	0.99	0.17	15,15,15,15	0
59	ZN	16	102	1/1	0.99	0.21	41,41,41,41	0
57	MG	1A	3161	1/1	0.99	0.17	27,27,27,27	0
57	MG	1A	3360	1/1	0.99	0.14	33,33,33,33	0
57	MG	1A	3029	1/1	0.99	0.22	31,31,31,31	0
57	MG	1A	3150	1/1	0.99	0.28	32,32,32,32	0
57	MG	1A	3978	1/1	0.99	0.10	40,40,40,40	0
57	MG	1A	3003	1/1	0.99	0.15	28,28,28,28	0
57	MG	2A	3478	1/1	0.99	0.23	64,64,64,64	0
60	SF4	1d	302	8/8	0.99	0.16	57,60,69,76	0
57	MG	1A	4073	1/1	0.99	0.20	28,28,28,28	0
57	MG	2A	3686	1/1	0.99	0.17	30,30,30,30	0
57	MG	1a	1805	1/1	1.00	0.10	40,40,40,40	0
57	MG	1A	3592	1/1	1.00	0.15	37,37,37,37	0
59	ZN	1n	103	1/1	1.00	0.15	63,63,63,63	0
59	ZN	15	110	1/1	1.00	0.27	47,47,47,47	0

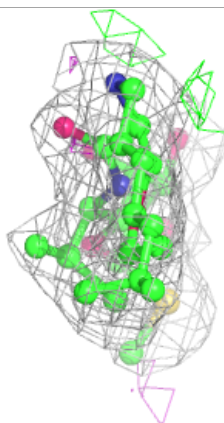
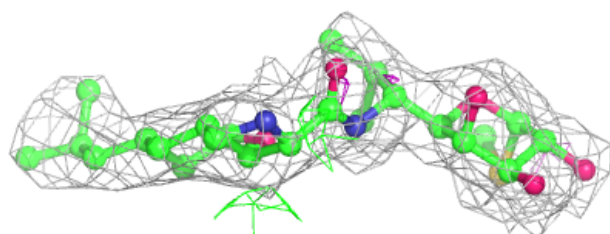
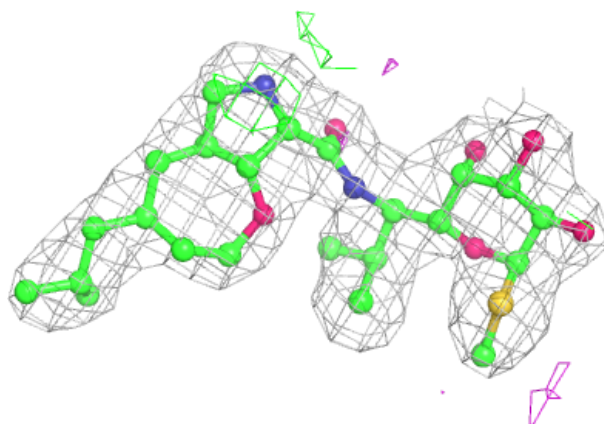
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 6IF 2A 3731:

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

**Electron density around 6IF 1A 4109:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.