



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2020 – 09:30 PM BST

PDB ID : 7JQM
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with Bac7-002, mRNA, and deacylated P-site tRNA at 3.05Å resolution
Authors : Mardirossian, M.; Sola, R.; Beckert, B.; Valencic, E.; Collis, D.W.P.; Borisek, J.; Armas, F.; Di Stasi, A.; Buchmann, J.; Syroegin, E.A.; Polikanov, Y.S.; Magistrato, A.; Hilpert, K.; Wilson, D.N.; Scocchi, M.
Deposited on : 2020-08-11
Resolution : 3.05 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	:	2.13
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)	:	2.13

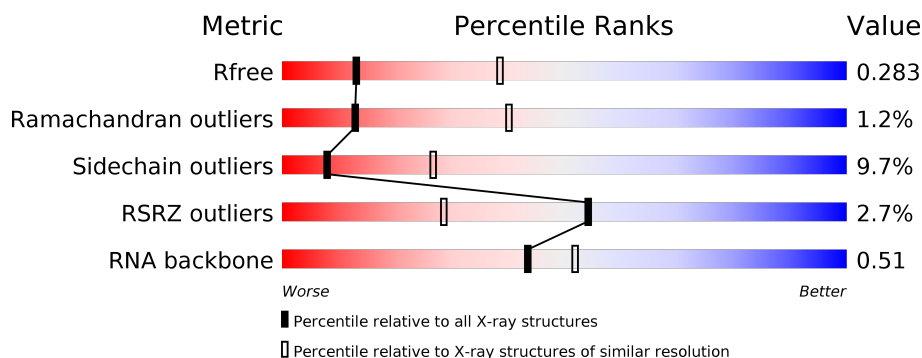
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.05 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.




















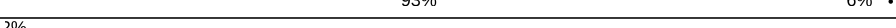

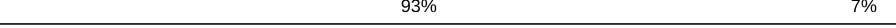
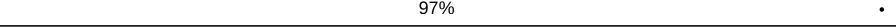




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1754 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)
RNA backbone	3102	1036 (3.32-2.80)

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

Mol	Chain	Length	Quality of chain
1	1A	2915	<div> <div>81%</div> <div>17%</div> <div>•</div> </div>
1	2A	2915	<div> <div>78%</div> <div>18%</div> <div>•</div> </div>
2	1B	121	<div> <div>89%</div> <div>10%</div> <div>•</div> </div>
2	2B	121	<div> <div>71%</div> <div>28%</div> <div>•</div> </div>
3	1D	276	<div> <div>3%</div> <div>91%</div> <div>9%</div> </div>
3	2D	276	<div> <div>3%</div> <div>91%</div> <div>8%</div> </div>

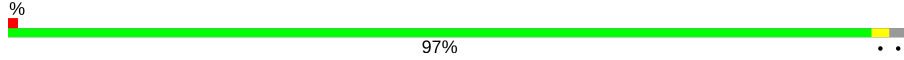



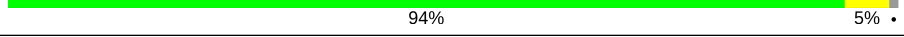
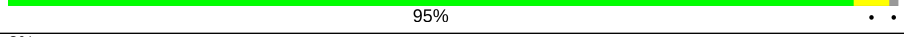
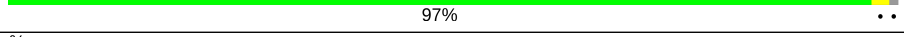

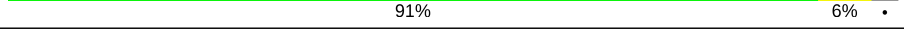


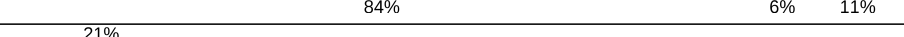

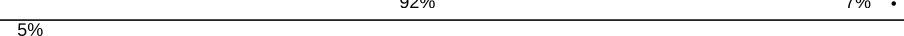
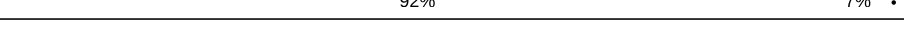

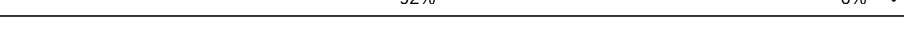

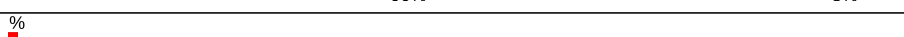
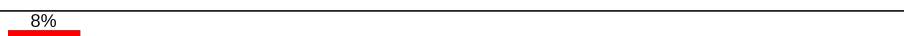

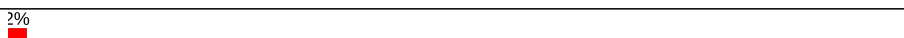
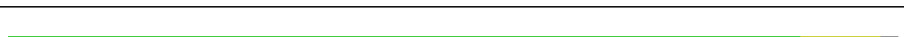


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Mol	Chain	Length	Quality of chain
4	1E	206	 90% 9% .
4	2E	206	 90% 9% .
5	1F	210	 90% 7% .
5	2F	210	 2% 86% 10% .
6	1G	182	 91% 8% .
6	2G	182	 18% 87% 11% ..
7	1H	180	 87% 9% .
7	2H	180	 11% 92% 5% .
8	1I	148	 89% 9% .
8	2I	148	 2% 87% 11% .
9	1N	140	 91% 9% .
9	2N	140	 6% 91% 9% .
10	1O	122	 96% .
10	2O	122	 96% .
11	1P	150	 91% 8% .
11	2P	150	 7% 89% 9% ..
12	1Q	141	 93% 6% .
12	2Q	141	 2% 89% 11% .
13	1R	118	 93% 7% .
13	2R	118	 97% .
14	1S	112	 87% 12% .
14	2S	112	 6% 87% 12% .
15	1T	146	 84% 5% 10%
15	2T	146	 82% 8% 10%
16	1U	118	 95% ..

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Mol	Chain	Length	Quality of chain
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	
28	26	54	

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Mol	Chain	Length	Quality of chain
29	17	49	<div> <div>4%</div> <div>90%</div> <div>8%</div> <div>.</div> </div>
29	27	49	<div> <div>6%</div> <div>90%</div> <div>8%</div> <div>.</div> </div>
30	18	65	<div> <div>3%</div> <div>92%</div> <div>6%</div> <div>.</div> </div>
30	28	65	<div> <div>15%</div> <div>94%</div> <div>5%</div> <div>.</div> </div>
31	19	37	<div> <div>97%</div> <div>.</div> </div>
31	29	37	<div> <div>5%</div> <div>92%</div> <div>8%</div> </div>
32	1a	1521	<div> <div>80%</div> <div>18%</div> <div>.</div> </div>
32	2a	1521	<div> <div>%</div> <div>78%</div> <div>20%</div> <div>..</div> </div>
33	1b	256	<div> <div>78%</div> <div>12%</div> <div>10%</div> </div>
33	2b	256	<div> <div>10%</div> <div>81%</div> <div>9%</div> <div>10%</div> </div>
34	1c	239	<div> <div>3%</div> <div>78%</div> <div>8%</div> <div>14%</div> </div>
34	2c	239	<div> <div>9%</div> <div>77%</div> <div>8%</div> <div>14%</div> </div>
35	1d	209	<div> <div>2%</div> <div>89%</div> <div>10%</div> </div>
35	2d	209	<div> <div>7%</div> <div>91%</div> <div>8%</div> </div>
36	1e	162	<div> <div>6%</div> <div>85%</div> <div>7%</div> <div>9%</div> </div>
36	2e	162	<div> <div>15%</div> <div>81%</div> <div>10%</div> <div>9%</div> </div>
37	1f	101	<div> <div>92%</div> <div>7%</div> <div>.</div> </div>
37	2f	101	<div> <div>91%</div> <div>8%</div> <div>.</div> </div>
38	1g	156	<div> <div>4%</div> <div>89%</div> <div>10%</div> <div>..</div> </div>
38	2g	156	<div> <div>10%</div> <div>89%</div> <div>10%</div> <div>.</div> </div>
39	1h	138	<div> <div>2%</div> <div>90%</div> <div>9%</div> <div>.</div> </div>
39	2h	138	<div> <div>14%</div> <div>93%</div> <div>7%</div> <div>.</div> </div>
40	1i	128	<div> <div>3%</div> <div>93%</div> <div>6%</div> <div>.</div> </div>
40	2i	128	<div> <div>23%</div> <div>91%</div> <div>7%</div> <div>..</div> </div>
41	1j	105	<div> <div>2%</div> <div>86%</div> <div>7%</div> <div>8%</div> </div>





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Mol	Chain	Length	Quality of chain
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	
53	2v	24	

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Mol	Chain	Length	Quality of chain
54	1x	77	
54	2x	77	
55	1z	16	
55	2z	16	

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
56	MG	1A	3150	-	-	-	X
56	MG	1A	3151	-	-	-	X
56	MG	1A	3152	-	-	-	X
56	MG	1A	3407	-	-	-	X
56	MG	1E	305	-	-	-	X
56	MG	2A	3254	-	-	-	X
56	MG	2A	3312	-	-	-	X

2 Entry composition [i](#)

There are 60 unique types of molecules in this entry. The entry contains 290774 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	76	Total	C	N	O	S	0	0	0
			604	373	128	102	1			
22	20	76	Total	C	N	O	S	0	0	0
			604	373	128	102	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 P-site tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	1x	76	Total	C	N	O	P	S	0	0
			1625	725	294	529	76	1		
54	2x	76	Total	C	N	O	P	S	0	0
			1625	725	294	529	76	1		

- Molecule 55 is a protein called Bac7-002.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
55	1z	16	Total	C	N	O	0	0	0
			147	93	38	16			
55	2z	16	Total	C	N	O	0	0	0
			141	90	35	16			

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2E	5	Total	Mg	0	0
			5	5		
56	17	6	Total	Mg	0	0
			6	6		
56	1z	1	Total	Mg	0	0
			1	1		
56	2d	1	Total	Mg	0	0
			1	1		
56	1T	2	Total	Mg	0	0
			2	2		
56	1N	3	Total	Mg	0	0
			3	3		
56	20	1	Total	Mg	0	0
			1	1		
56	18	4	Total	Mg	0	0
			4	4		
56	2W	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1Y	1	Total 1	Mg 1	0	0
56	13	3	Total 3	Mg 3	0	0
56	1f	2	Total 2	Mg 2	0	0
56	1P	5	Total 5	Mg 5	0	0
56	2B	12	Total 12	Mg 12	0	0
56	23	2	Total 2	Mg 2	0	0
56	1E	8	Total 8	Mg 8	0	0
56	2l	2	Total 2	Mg 2	0	0
56	2F	4	Total 4	Mg 4	0	0
56	28	3	Total 3	Mg 3	0	0
56	1W	6	Total 6	Mg 6	0	0
56	1A	848	Total 848	Mg 848	0	0
56	21	1	Total 1	Mg 1	0	0
56	1n	2	Total 2	Mg 2	0	0
56	2P	3	Total 3	Mg 3	0	0
56	1X	3	Total 3	Mg 3	0	0
56	12	2	Total 2	Mg 2	0	0
56	1S	1	Total 1	Mg 1	0	0
56	25	2	Total 2	Mg 2	0	0
56	2T	2	Total 2	Mg 2	0	0
56	1D	8	Total 8	Mg 8	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2N	1	Total 1	Mg 1	0	0
56	1e	2	Total 2	Mg 2	0	0
56	1I	1	Total 1	Mg 1	0	0
56	2f	1	Total 1	Mg 1	0	0
56	1V	5	Total 5	Mg 5	0	0
56	2v	2	Total 2	Mg 2	0	0
56	26	1	Total 1	Mg 1	0	0
56	1a	167	Total 167	Mg 167	0	0
56	2Q	2	Total 2	Mg 2	0	0
56	15	5	Total 5	Mg 5	0	0
56	1x	10	Total 10	Mg 10	0	0
56	2j	1	Total 1	Mg 1	0	0
56	1R	6	Total 6	Mg 6	0	0
56	1s	1	Total 1	Mg 1	0	0
56	1m	1	Total 1	Mg 1	0	0
56	1G	4	Total 4	Mg 4	0	0
56	2O	1	Total 1	Mg 1	0	0
56	11	2	Total 2	Mg 2	0	0
56	1d	1	Total 1	Mg 1	0	0
56	2r	1	Total 1	Mg 1	0	0
56	1H	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2q	2	Total 2	Mg 2	0	0
56	2Y	1	Total 1	Mg 1	0	0
56	1v	1	Total 1	Mg 1	0	0
56	2x	3	Total 3	Mg 3	0	0
56	2R	1	Total 1	Mg 1	0	0
56	1Z	3	Total 3	Mg 3	0	0
56	2D	2	Total 2	Mg 2	0	0
56	14	1	Total 1	Mg 1	0	0
56	2k	1	Total 1	Mg 1	0	0
56	1U	6	Total 6	Mg 6	0	0
56	1O	1	Total 1	Mg 1	0	0
56	27	2	Total 2	Mg 2	0	0
56	19	1	Total 1	Mg 1	0	0
56	1l	3	Total 3	Mg 3	0	0
56	2V	2	Total 2	Mg 2	0	0
56	1F	12	Total 12	Mg 12	0	0
56	10	5	Total 5	Mg 5	0	0
56	2t	1	Total 1	Mg 1	0	0
56	1Q	4	Total 4	Mg 4	0	0
56	2A	625	Total 625	Mg 625	0	0
56	1h	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2Z	1	Total 1	Mg 1	0	0
56	1B	25	Total 25	Mg 25	0	0
56	2a	145	Total 145	Mg 145	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1Y	1	Total 1	Zn 1	0	0
57	14	1	Total 1	Zn 1	0	0
57	1n	1	Total 1	Zn 1	0	0
57	15	1	Total 1	Zn 1	0	0
57	29	1	Total 1	Zn 1	0	0
57	19	1	Total 1	Zn 1	0	0
57	26	1	Total 1	Zn 1	0	0
57	25	1	Total 1	Zn 1	0	0
57	24	1	Total 1	Zn 1	0	0
57	2n	1	Total 1	Zn 1	0	0
57	2Y	1	Total 1	Zn 1	0	0
57	16	1	Total 1	Zn 1	0	0

- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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

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

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

- Molecule 60 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1A	1222	Total	O	0	0
			1222	1222		
60	1B	27	Total	O	0	0
			27	27		
60	1D	21	Total	O	0	0
			21	21		
60	1E	11	Total	O	0	0
			11	11		
60	1F	9	Total	O	0	0
			9	9		
60	1N	1	Total	O	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1O	1	Total 1	O 1	0	0
60	1P	14	Total 14	O 14	0	0
60	1Q	2	Total 2	O 2	0	0
60	1R	3	Total 3	O 3	0	0
60	1S	2	Total 2	O 2	0	0
60	1T	4	Total 4	O 4	0	0
60	1U	4	Total 4	O 4	0	0
60	1V	4	Total 4	O 4	0	0
60	1W	3	Total 3	O 3	0	0
60	10	2	Total 2	O 2	0	0
60	11	2	Total 2	O 2	0	0
60	12	2	Total 2	O 2	0	0
60	13	2	Total 2	O 2	0	0
60	18	2	Total 2	O 2	0	0
60	1a	26	Total 26	O 26	0	0
60	1d	1	Total 1	O 1	0	0
60	1z	1	Total 1	O 1	0	0
60	2A	416	Total 416	O 416	0	0
60	2B	3	Total 3	O 3	0	0
60	2D	12	Total 12	O 12	0	0
60	2E	4	Total 4	O 4	0	0

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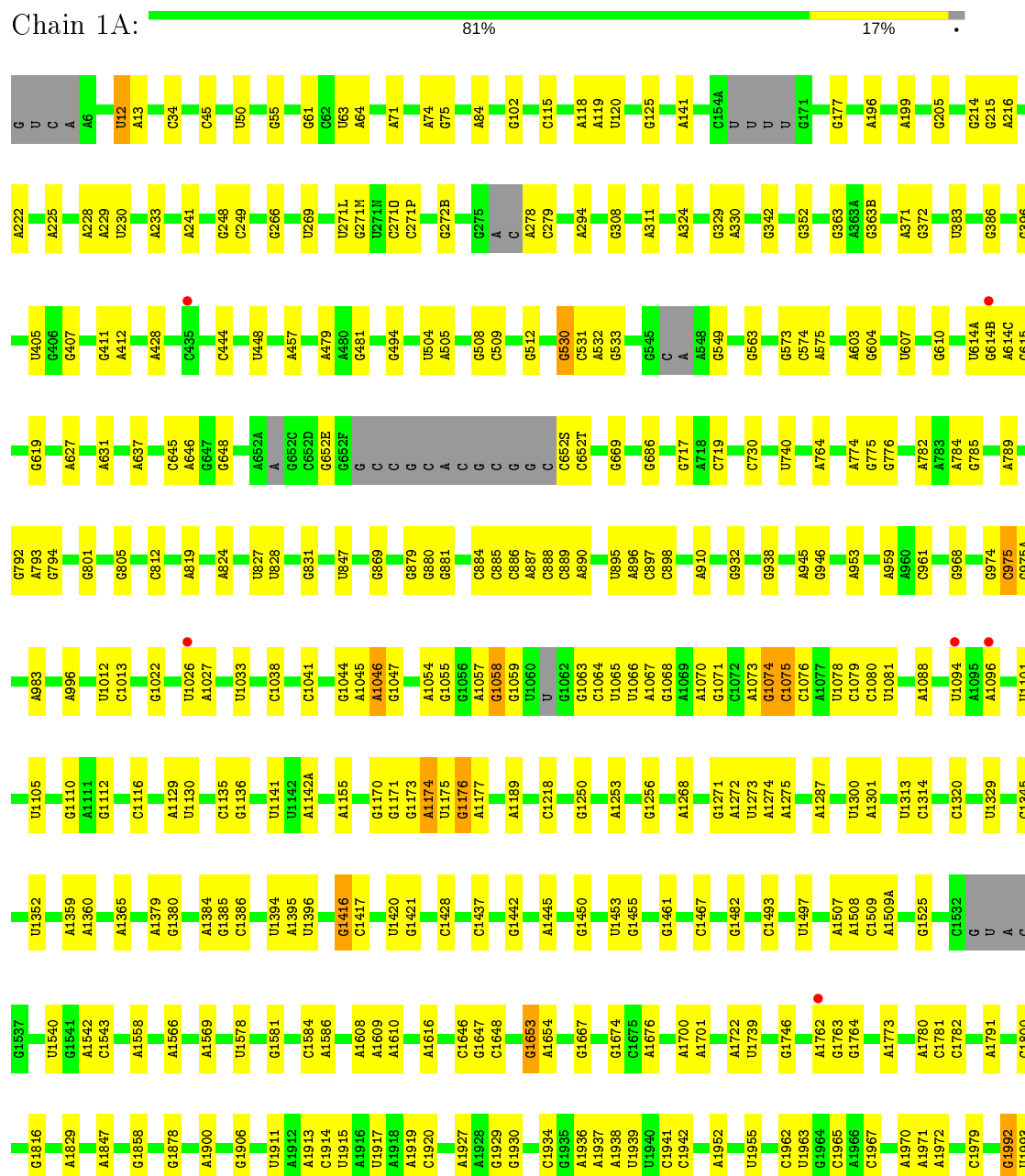
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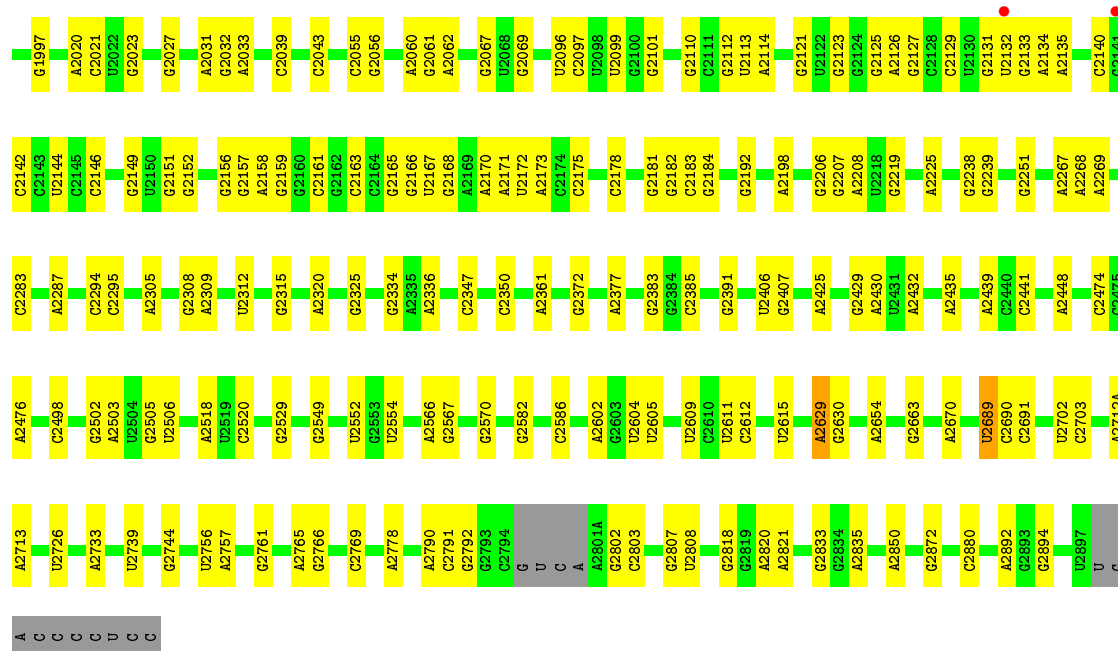
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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60	2I	1	Total 1	O 1	0	0
60	2O	3	Total 3	O 3	0	0
60	2P	4	Total 4	O 4	0	0
60	2Q	1	Total 1	O 1	0	0
60	2R	1	Total 1	O 1	0	0
60	2T	1	Total 1	O 1	0	0
60	2V	1	Total 1	O 1	0	0
60	2W	2	Total 2	O 2	0	0
60	20	1	Total 1	O 1	0	0
60	21	2	Total 2	O 2	0	0
60	28	2	Total 2	O 2	0	0
60	2a	17	Total 17	O 17	0	0
60	2l	1	Total 1	O 1	0	0
60	2n	1	Total 1	O 1	0	0
60	2t	1	Total 1	O 1	0	0
60	2x	1	Total 1	O 1	0	0

3 Residue-property plots [i](#)


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

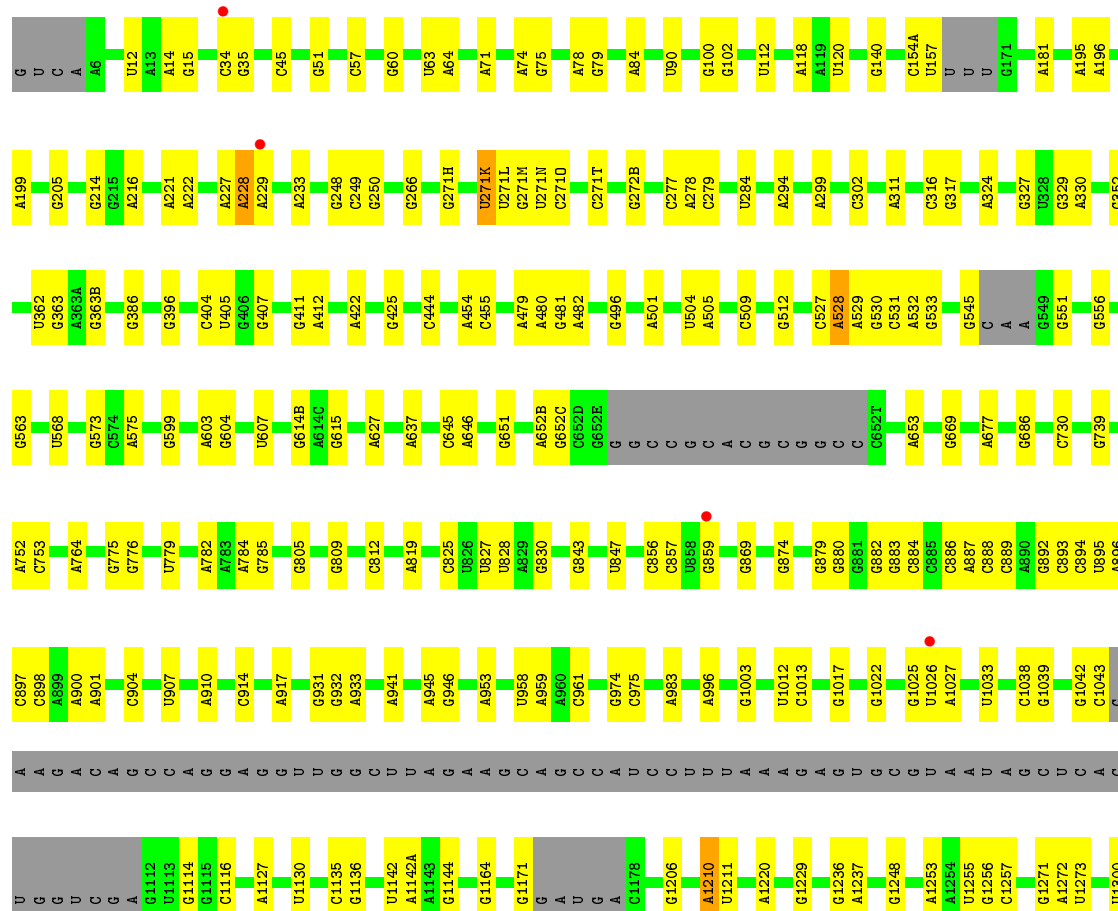
• Molecule 1: 23S Ribosomal RNA

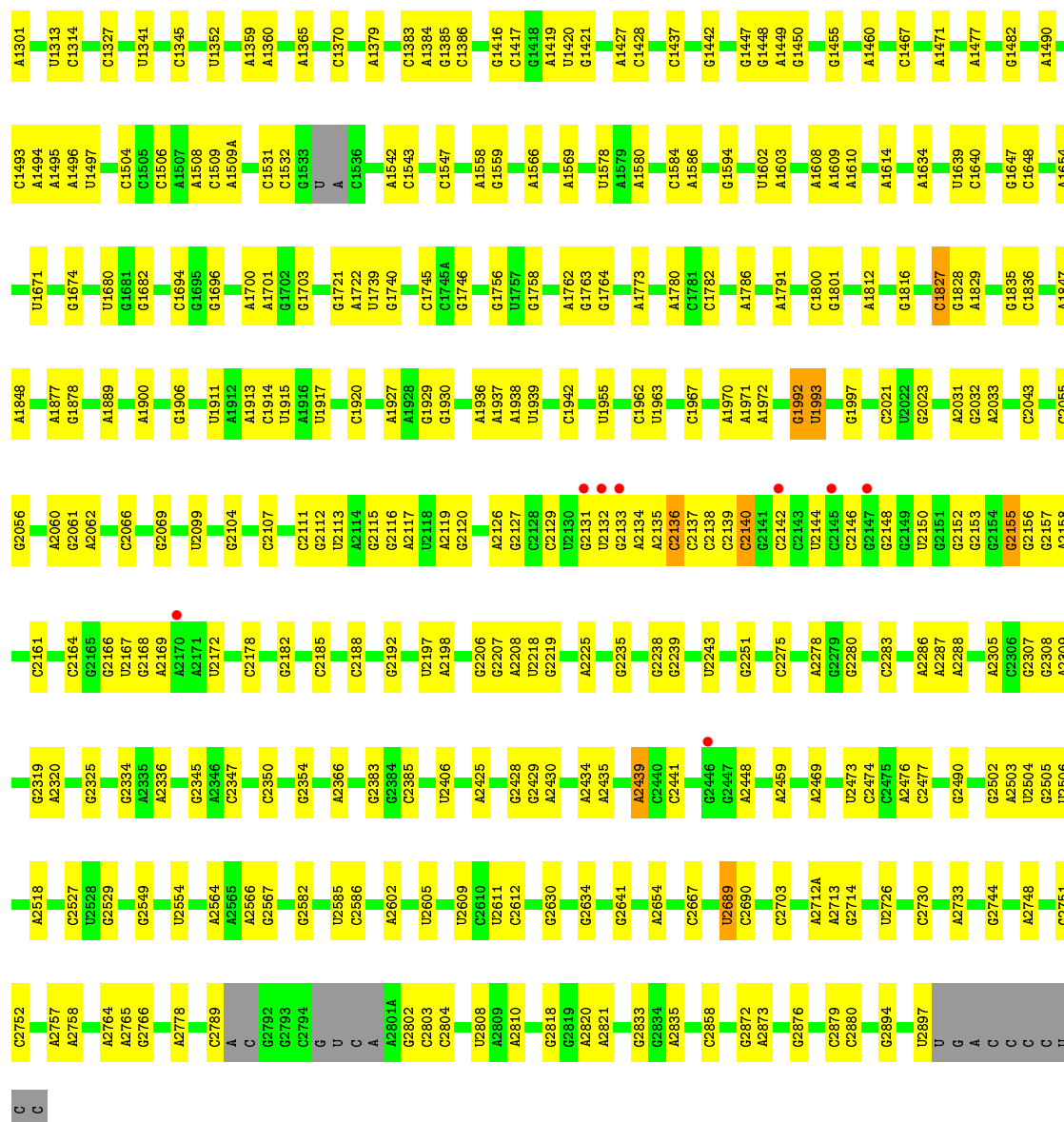




- Molecule 1: 23S Ribosomal RNA

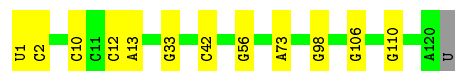
Chain 2A:  78% 18%





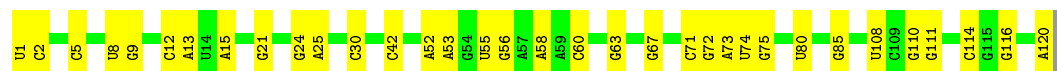
- Molecule 2: 5S Ribosomal RNA

Chain 1B: 89% 10%

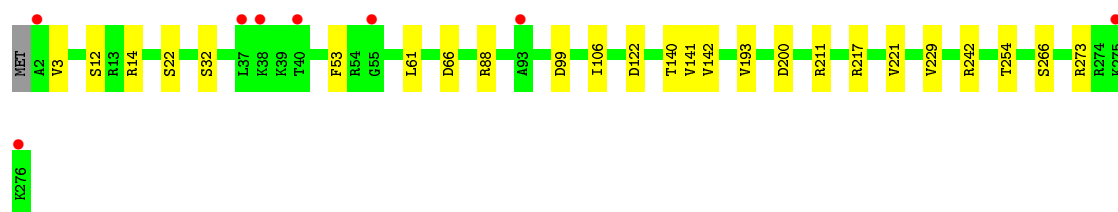
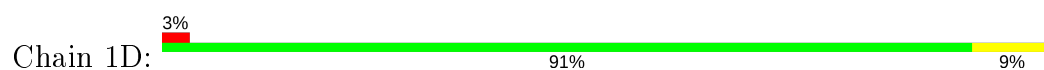


- Molecule 2: 5S Ribosomal RNA

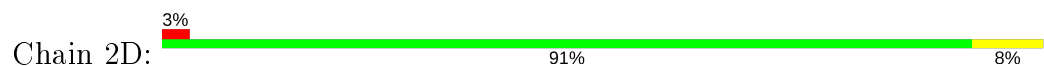
Chain 2B: 71% 28%



- Molecule 3: 50S ribosomal protein L2



- Molecule 3: 50S ribosomal protein L2



- Molecule 4: 50S ribosomal protein L3



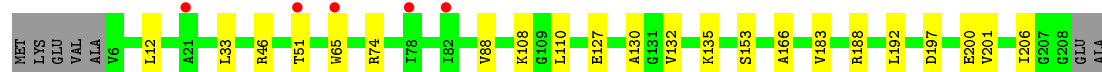
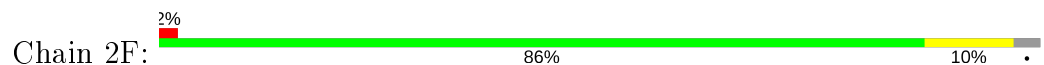
- Molecule 4: 50S ribosomal protein L3



- Molecule 5: 50S ribosomal protein L4



- Molecule 5: 50S ribosomal protein L4

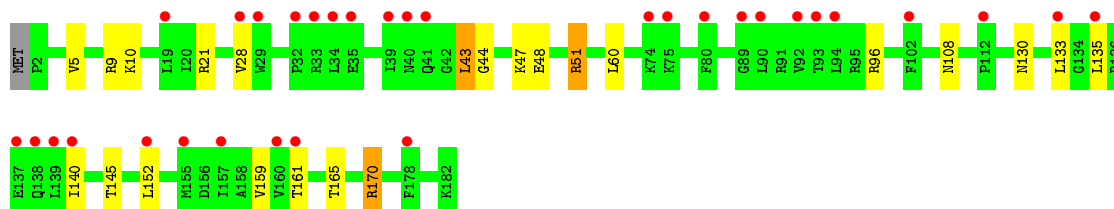
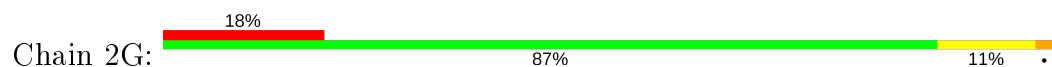


- Molecule 6: 50S ribosomal protein L5

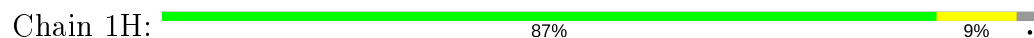




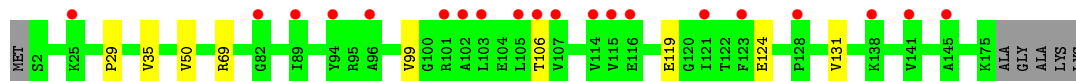
- Molecule 6: 50S ribosomal protein L5



- Molecule 7: 50S ribosomal protein L6



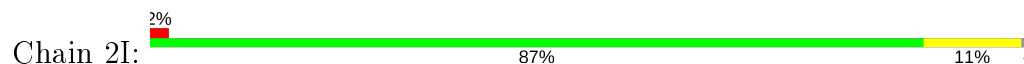
- Molecule 7: 50S ribosomal protein L6



- Molecule 8: 50S ribosomal protein L9



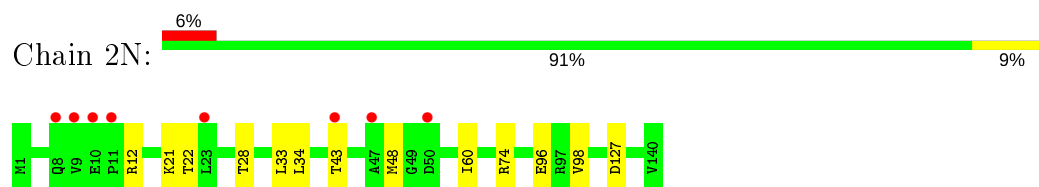
- Molecule 8: 50S ribosomal protein L9



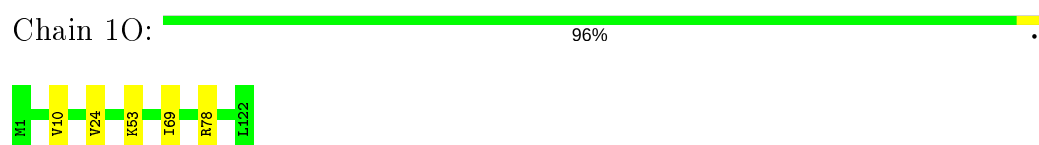
- Molecule 9: 50S ribosomal protein L13



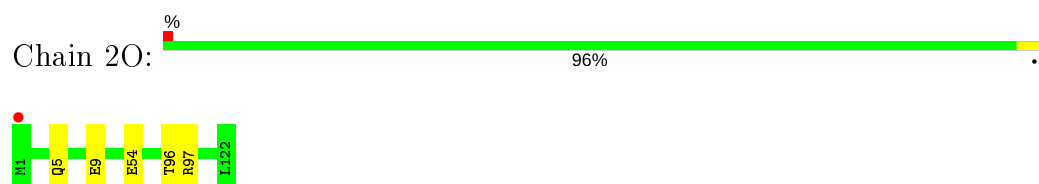
- Molecule 9: 50S ribosomal protein L13



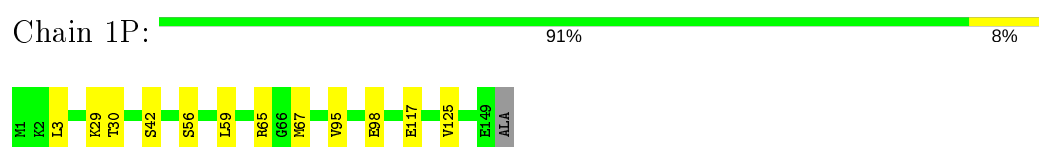
- Molecule 10: 50S ribosomal protein L14



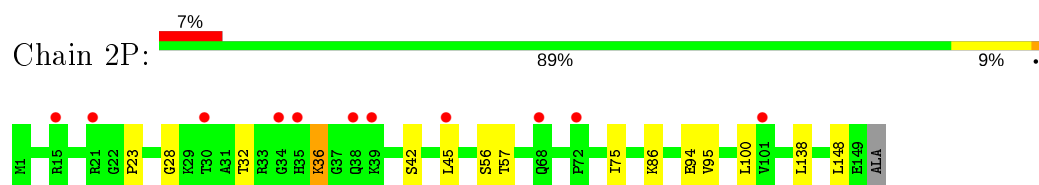
- Molecule 10: 50S ribosomal protein L14



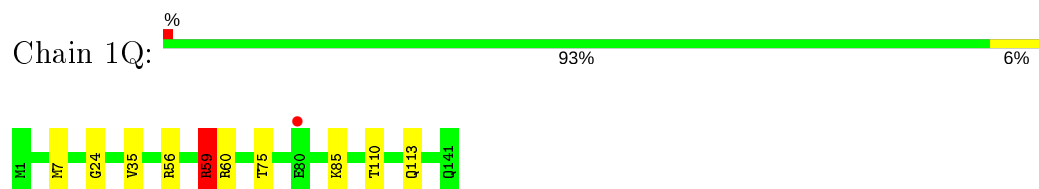
- Molecule 11: 50S ribosomal protein L15



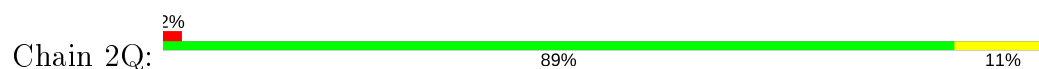
- Molecule 11: 50S ribosomal protein L15

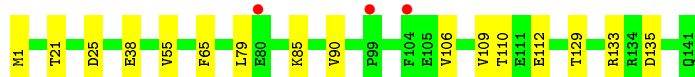


- Molecule 12: 50S ribosomal protein L16



- Molecule 12: 50S ribosomal protein L16





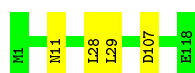
- Molecule 13: 50S ribosomal protein L17

Chain 1R: 93% 7%



- Molecule 13: 50S ribosomal protein L17

Chain 2R: 97%



- Molecule 14: 50S ribosomal protein L18

Chain 1S: 87% 12%



- Molecule 14: 50S ribosomal protein L18

Chain 2S: 6% 87% 12%



- Molecule 15: 50S ribosomal protein L19

Chain 1T: 84% 5% 10%



- Molecule 15: 50S ribosomal protein L19

Chain 2T: % 82% 8% 10%

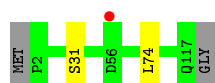


- Molecule 16: 50S ribosomal protein L20

Chain 1U: % 95%



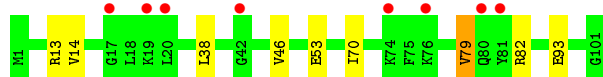
- Molecule 16: 50S ribosomal protein L20



- Molecule 17: 50S ribosomal protein L21



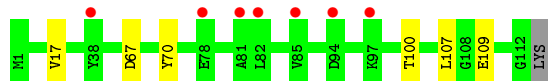
- Molecule 17: 50S ribosomal protein L21



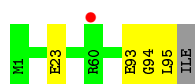
- Molecule 18: 50S ribosomal protein L22



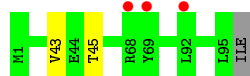
- Molecule 18: 50S ribosomal protein L22



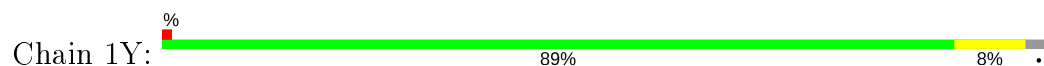
- Molecule 19: 50S ribosomal protein L23



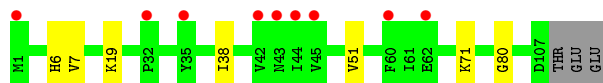
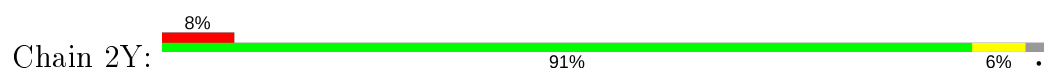
- Molecule 19: 50S ribosomal protein L23



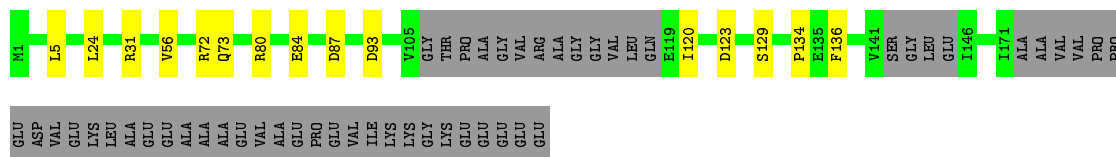
- Molecule 20: 50S ribosomal protein L24



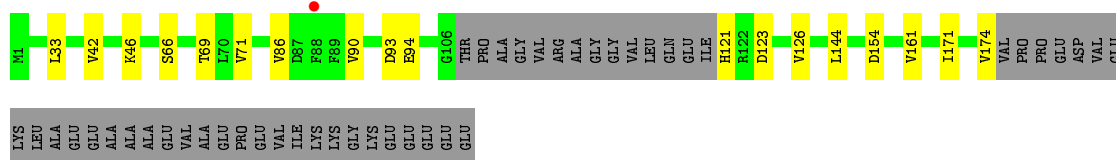
- Molecule 20: 50S ribosomal protein L24



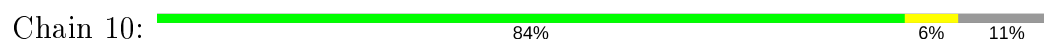
- Molecule 21: 50S ribosomal protein L25



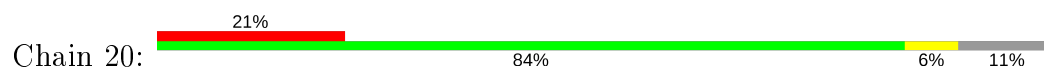
- Molecule 21: 50S ribosomal protein L25

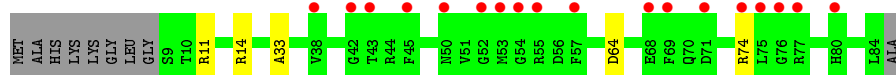


- Molecule 22: 50S ribosomal protein L27



- Molecule 22: 50S ribosomal protein L27





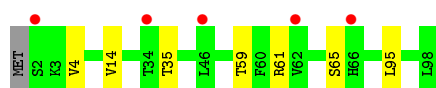
- Molecule 23: 50S ribosomal protein L28

Chain 11: 92% 7% .



- Molecule 23: 50S ribosomal protein L28

Chain 21: 5% 92% 7% .



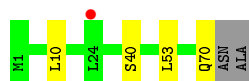
- Molecule 24: 50S ribosomal protein L29

Chain 12: 88% 10% .



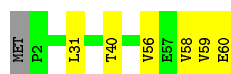
- Molecule 24: 50S ribosomal protein L29

Chain 22: % 92% 6% .



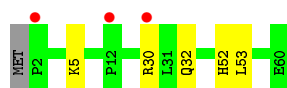
- Molecule 25: 50S ribosomal protein L30

Chain 13: 88% 10% .



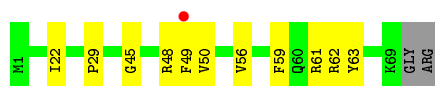
- Molecule 25: 50S ribosomal protein L30

Chain 23: 5% 90% 8% .

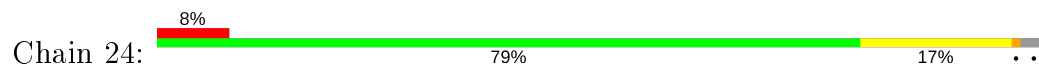


- Molecule 26: 50S ribosomal protein L31

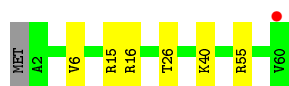
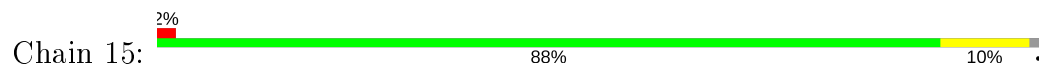
Chain 14: % 82% 15% .



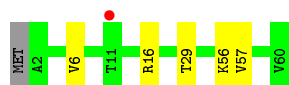
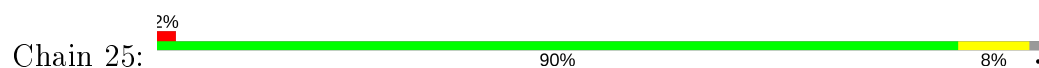
- Molecule 26: 50S ribosomal protein L31



- Molecule 27: 50S ribosomal protein L32



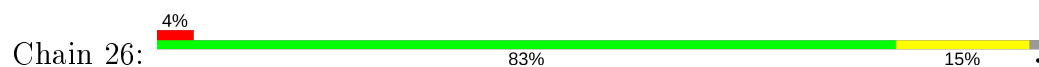
- Molecule 27: 50S ribosomal protein L32



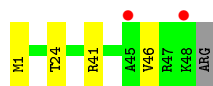
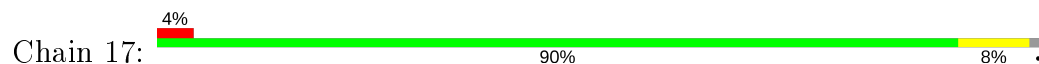
- Molecule 28: 50S ribosomal protein L33



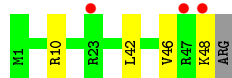
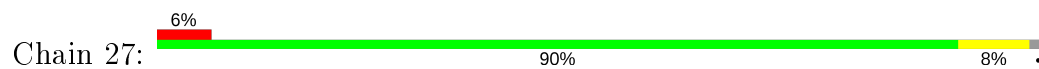
- Molecule 28: 50S ribosomal protein L33



- Molecule 29: 50S ribosomal protein L34



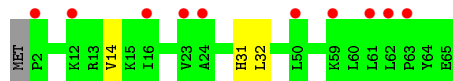
- Molecule 29: 50S ribosomal protein L34



- Molecule 30: 50S ribosomal protein L35



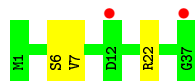
- Molecule 30: 50S ribosomal protein L35



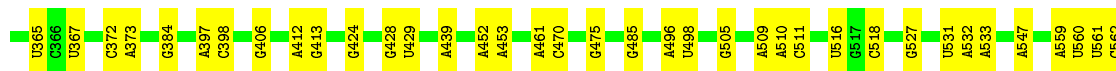
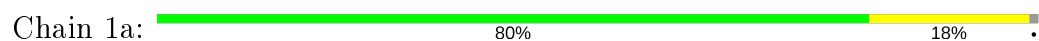
- Molecule 31: 50S ribosomal protein L36

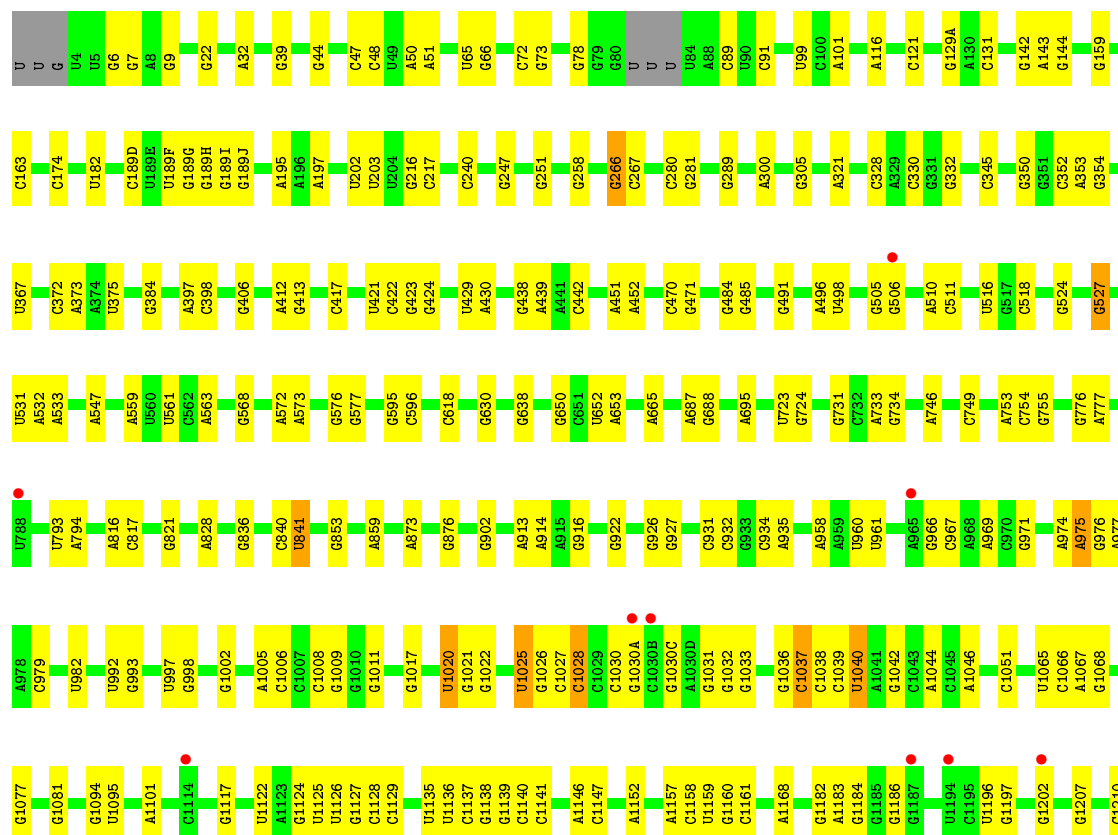


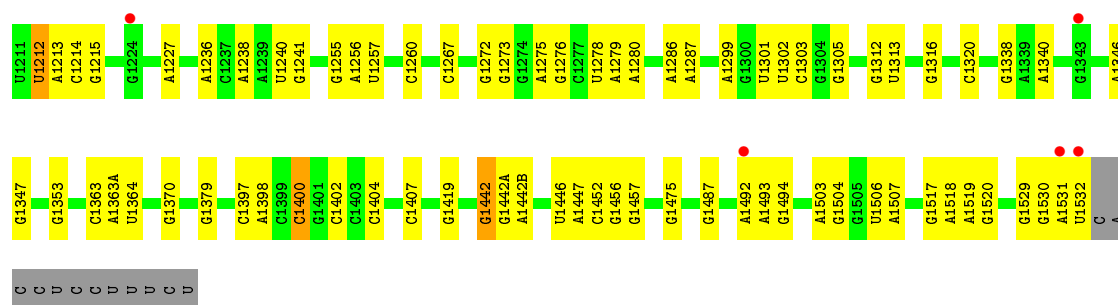
- Molecule 31: 50S ribosomal protein L36



- Molecule 32: 16S Ribosomal RNA

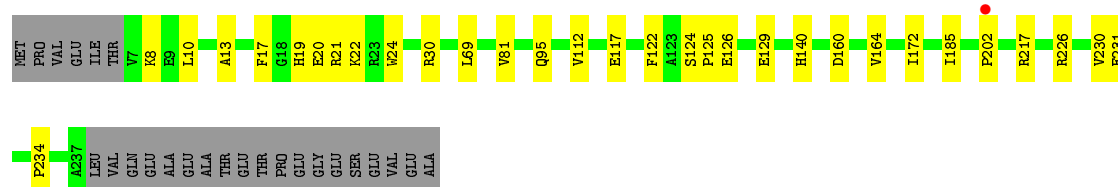






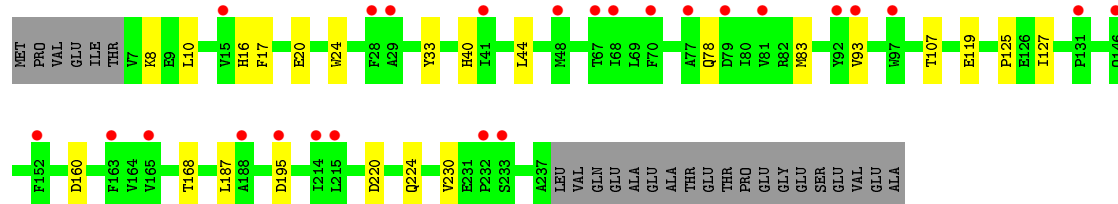
- Molecule 33: 30S ribosomal protein S2

Chain 1b: 78% 12% 10%



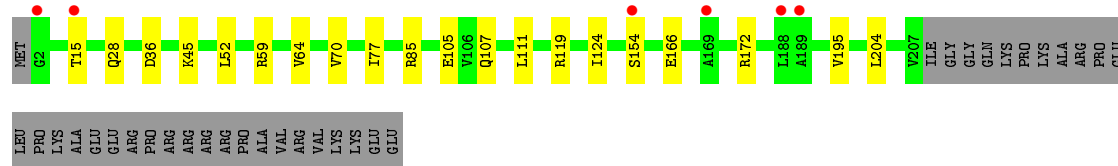
- Molecule 33: 30S ribosomal protein S2

Chain 2b: 10% 81% 9% 10%



- Molecule 34: 30S ribosomal protein S3

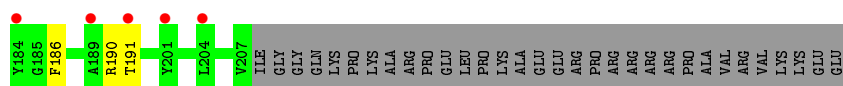
Chain 1c: 3% 78% 8% 14%



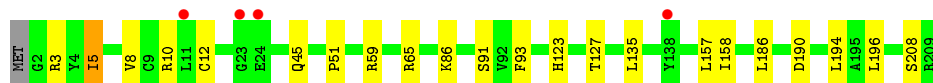
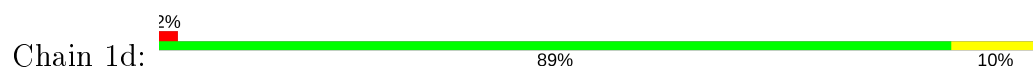
- Molecule 34: 30S ribosomal protein S3

Chain 2c: 9% 77% 8% 14%

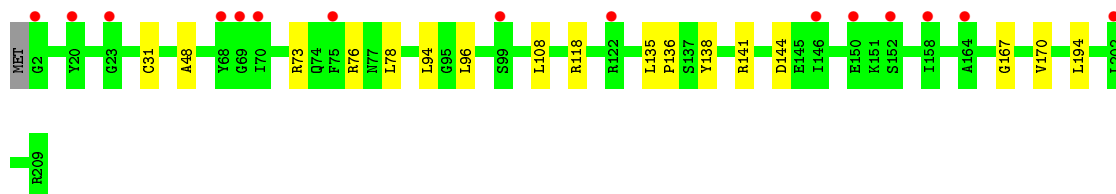




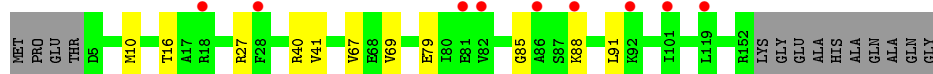
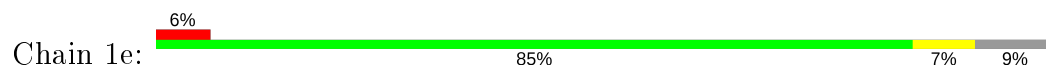
- Molecule 35: 30S ribosomal protein S4



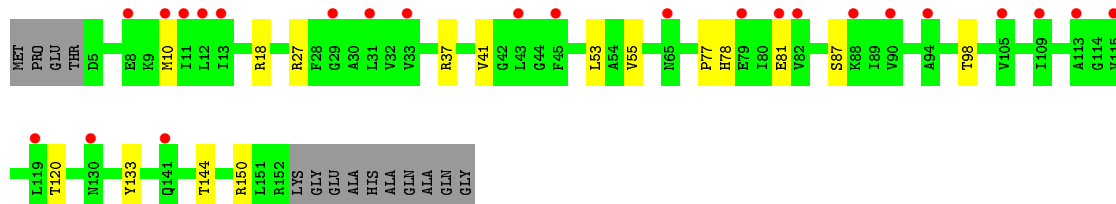
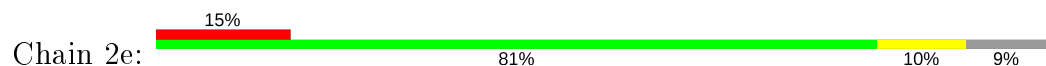
- Molecule 35: 30S ribosomal protein S4



- Molecule 36: 30S ribosomal protein S5



- Molecule 36: 30S ribosomal protein S5

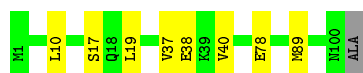


- Molecule 37: 30S ribosomal protein S6

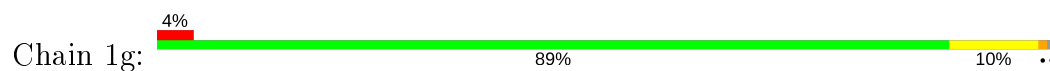


- Molecule 37: 30S ribosomal protein S6

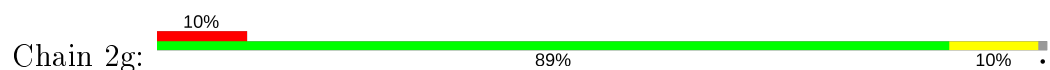




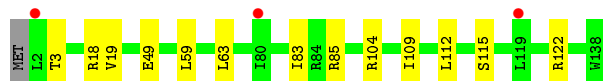
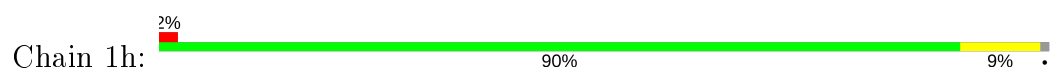
- Molecule 38: 30S ribosomal protein S7



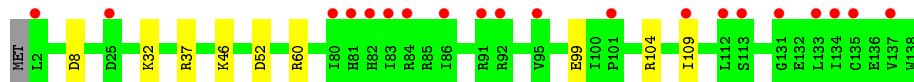
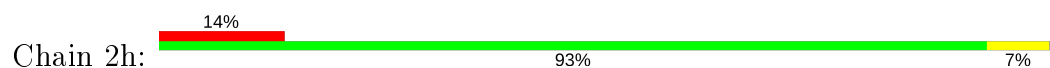
- Molecule 38: 30S ribosomal protein S7



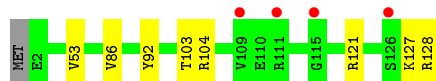
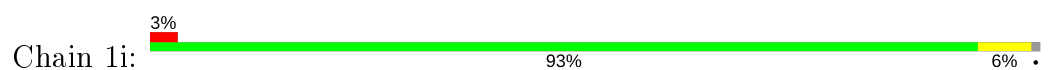
- Molecule 39: 30S ribosomal protein S8



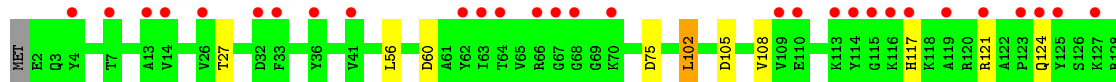
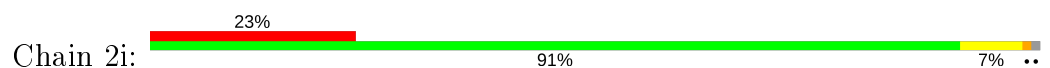
- Molecule 39: 30S ribosomal protein S8



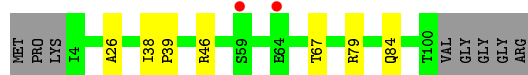
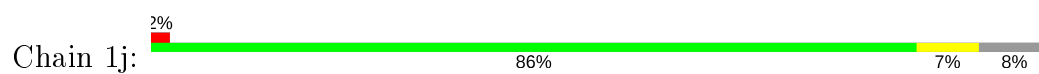
- Molecule 40: 30S ribosomal protein S9



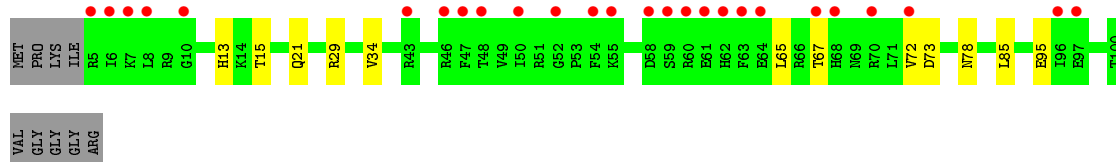
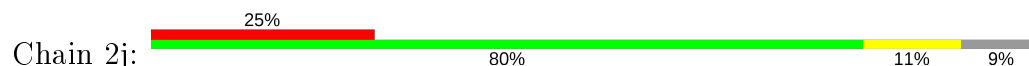
- Molecule 40: 30S ribosomal protein S9



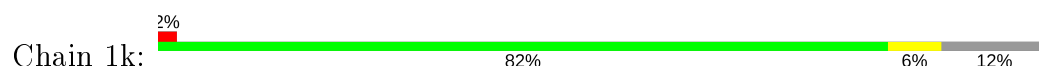
- Molecule 41: 30S ribosomal protein S10



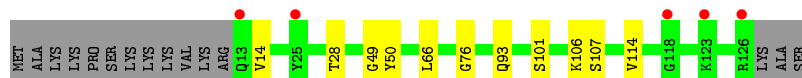
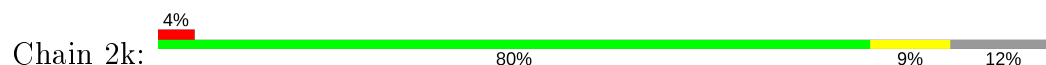
- Molecule 41: 30S ribosomal protein S10



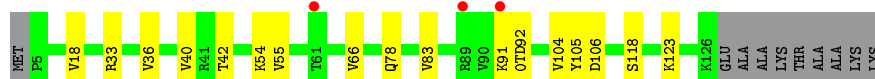
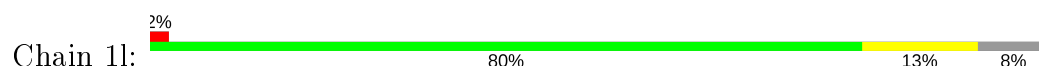
- Molecule 42: 30S ribosomal protein S11



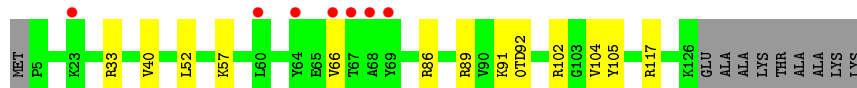
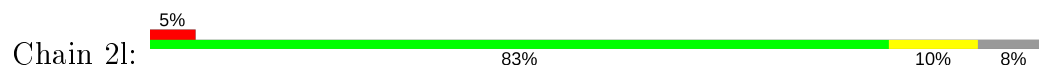
- Molecule 42: 30S ribosomal protein S11



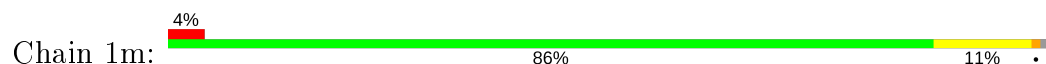
- Molecule 43: 30S ribosomal protein S12



- Molecule 43: 30S ribosomal protein S12

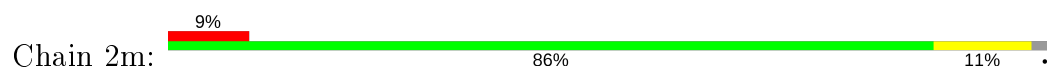


- Molecule 44: 30S ribosomal protein S13

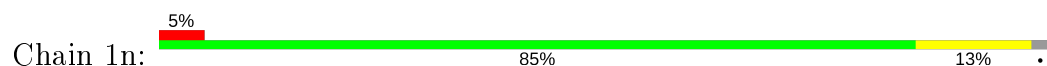




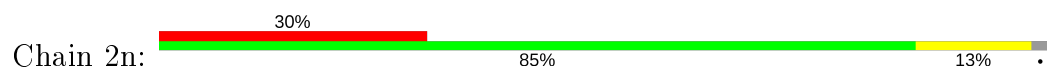
- Molecule 44: 30S ribosomal protein S13



- Molecule 45: 30S ribosomal protein S14 type Z



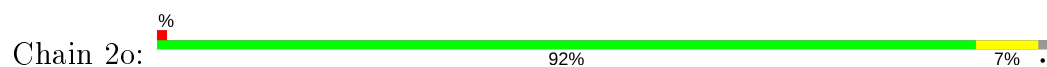
- Molecule 45: 30S ribosomal protein S14 type Z



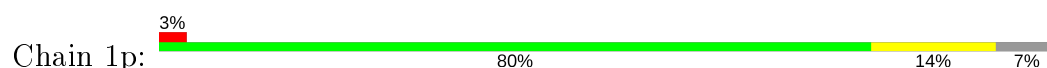
- Molecule 46: 30S ribosomal protein S15



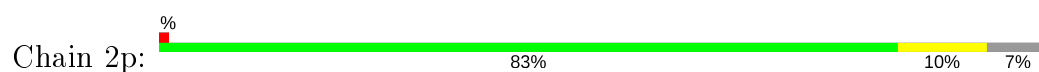
- Molecule 46: 30S ribosomal protein S15



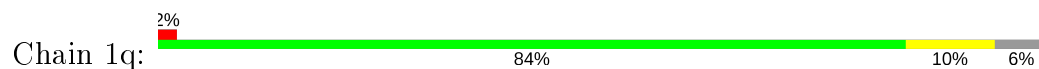
- Molecule 47: 30S ribosomal protein S16



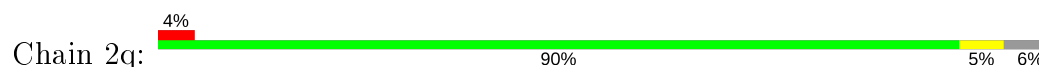
- Molecule 47: 30S ribosomal protein S16



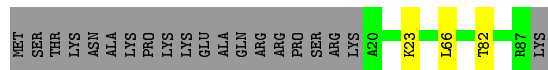
- Molecule 48: 30S ribosomal protein S17



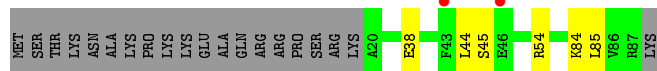
- Molecule 48: 30S ribosomal protein S17



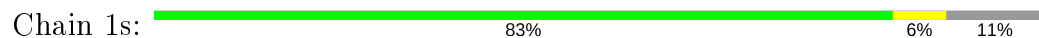
- Molecule 49: 30S ribosomal protein S18



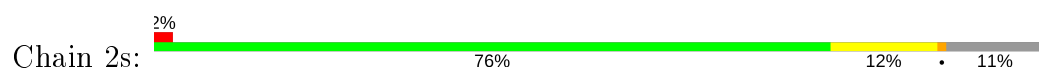
- Molecule 49: 30S ribosomal protein S18



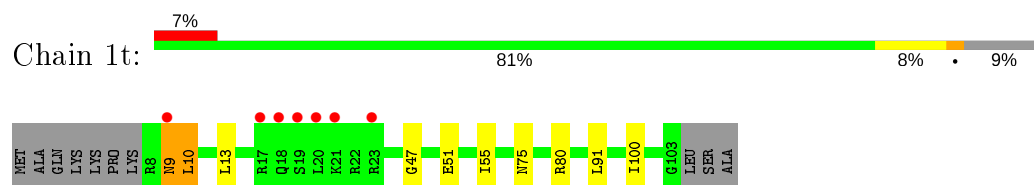
- Molecule 50: 30S ribosomal protein S19



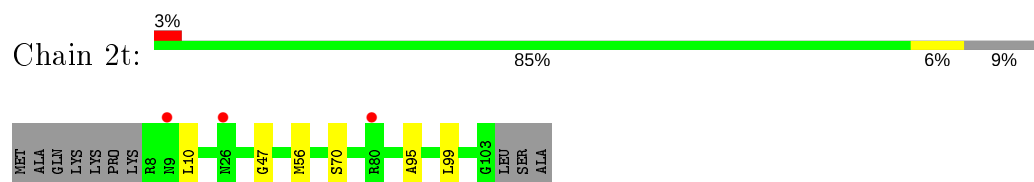
- Molecule 50: 30S ribosomal protein S19



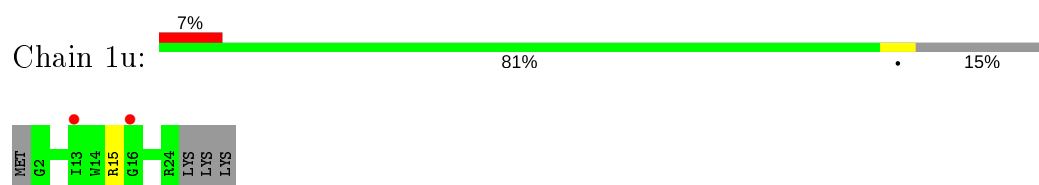
- Molecule 51: 30S ribosomal protein S20



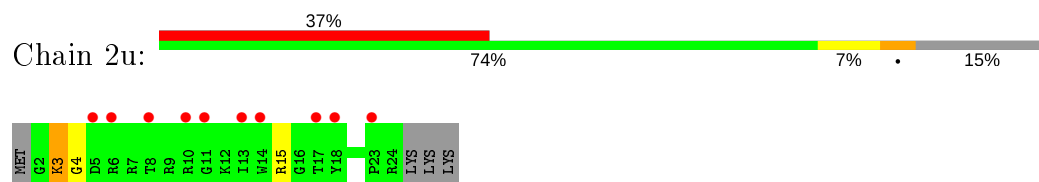
- Molecule 51: 30S ribosomal protein S20



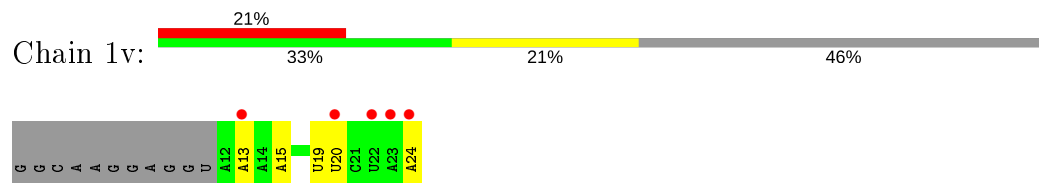
- Molecule 52: 30S ribosomal protein Thx



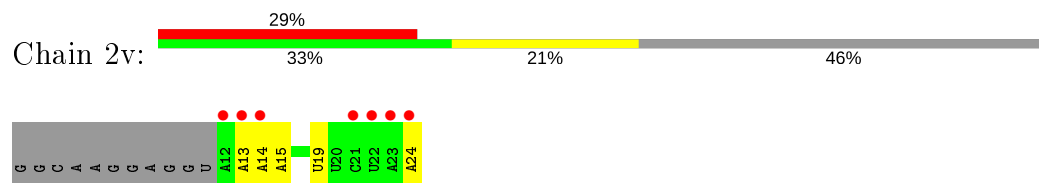
- Molecule 52: 30S ribosomal protein Thx



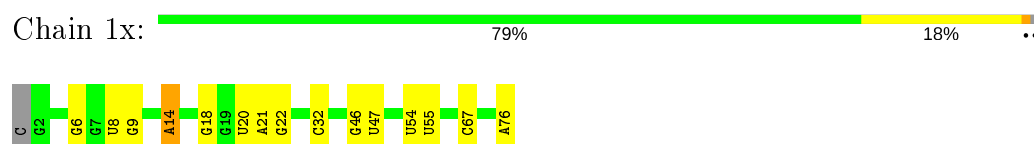
- Molecule 53: mRNA



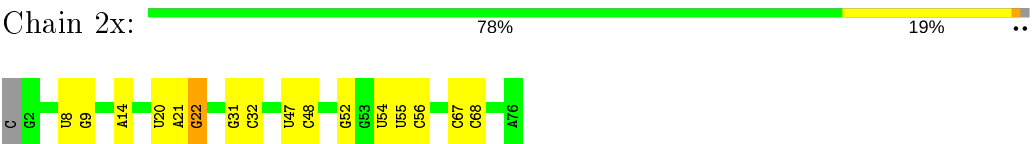
- Molecule 53: mRNA



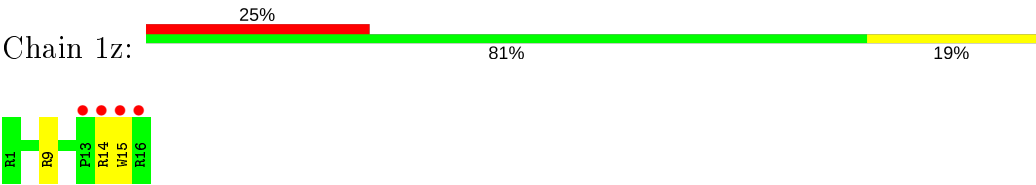
- Molecule 54: P-site tRNA



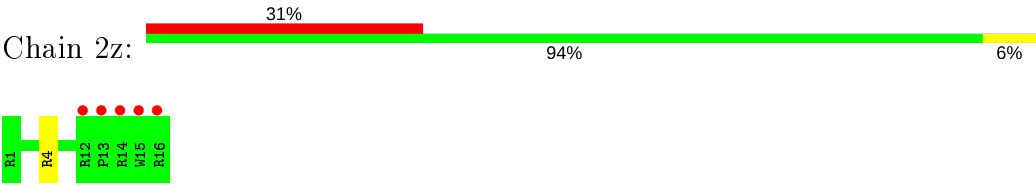
• Molecule 54: P-site tRNA



• Molecule 55: Bac7-002



• Molecule 55: Bac7-002



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	208.64Å 447.57Å 619.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	151.79 – 3.05 309.87 – 3.05	Depositor EDS
% Data completeness (in resolution range)	98.7 (151.79-3.05) 98.7 (309.87-3.05)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 3.07Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.227 , 0.283 0.226 , 0.283	Depositor DCC
R_{free} test set	53845 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	62.7	Xtriage
Anisotropy	0.294	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 61.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	290774	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, ZN, M2G, OMG, MA6, SF4, 0TD, MG, 2MA, 2MU, 2MG, 5MC, UR3, 4OC, 4SU, 7MG, K, PSU

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	0.48	0/69009	0.91	39/107712 (0.0%)
1	2A	0.39	0/67293	0.88	36/105034 (0.0%)
2	1B	0.44	1/2882 (0.0%)	0.85	0/4494
2	2B	0.42	1/2879 (0.0%)	0.92	1/4487 (0.0%)
3	1D	0.35	0/2186	0.55	0/2944
3	2D	0.31	0/2186	0.53	0/2944
4	1E	0.34	0/1592	0.53	0/2149
4	2E	0.31	0/1592	0.52	0/2149
5	1F	0.33	0/1619	0.50	0/2193
5	2F	0.31	0/1615	0.50	0/2188
6	1G	0.29	0/1448	0.49	0/1957
6	2G	0.29	0/1453	0.50	1/1963 (0.1%)
7	1H	0.30	0/1356	0.47	0/1834
7	2H	0.29	0/1356	0.46	0/1834
8	1I	0.30	0/1112	0.48	0/1514
8	2I	0.27	0/1079	0.49	0/1475
9	1N	0.31	0/1144	0.49	1/1543 (0.1%)
9	2N	0.30	0/1144	0.48	0/1543
10	1O	0.33	0/943	0.54	0/1269
10	2O	0.31	0/943	0.54	0/1269
11	1P	0.32	0/1152	0.54	0/1533
11	2P	0.31	0/1152	0.54	0/1533
12	1Q	0.32	0/1143	0.54	0/1527
12	2Q	0.30	0/1143	0.51	0/1527
13	1R	0.29	0/982	0.51	0/1312
13	2R	0.28	0/982	0.48	0/1312
14	1S	0.30	0/883	0.50	0/1176
14	2S	0.30	0/880	0.51	0/1172
15	1T	0.30	0/1105	0.50	0/1477
15	2T	0.29	0/1097	0.49	0/1468
16	1U	0.34	0/977	0.47	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.29	0/977	0.45	0/1301
17	1V	0.33	0/782	0.53	0/1049
17	2V	0.29	0/782	0.48	0/1049
18	1W	0.32	0/897	0.48	0/1205
18	2W	0.30	0/897	0.49	0/1205
19	1X	0.35	0/764	0.52	0/1025
19	2X	0.29	0/764	0.47	0/1025
20	1Y	0.31	0/819	0.52	0/1095
20	2Y	0.30	0/819	0.50	0/1095
21	1Z	0.31	0/1267	0.50	0/1717
21	2Z	0.31	0/1299	0.49	0/1763
22	10	0.34	0/612	0.53	0/816
22	20	0.30	0/612	0.49	0/816
23	11	0.32	0/762	0.50	0/1014
23	21	0.32	0/762	0.51	0/1014
24	12	0.32	0/590	0.46	0/781
24	22	0.29	0/590	0.40	0/781
25	13	0.30	0/474	0.52	0/635
25	23	0.28	0/469	0.47	0/630
26	14	0.33	0/565	0.50	0/761
26	24	0.34	0/545	0.56	0/737
27	15	0.32	0/469	0.50	0/635
27	25	0.34	0/469	0.48	0/635
28	16	0.35	0/460	0.53	0/613
28	26	0.31	0/456	0.49	0/608
29	17	0.32	0/426	0.53	0/561
29	27	0.32	0/426	0.50	0/561
30	18	0.32	0/525	0.52	0/691
30	28	0.31	0/525	0.50	0/691
31	19	0.35	0/310	0.52	0/407
31	29	0.29	0/310	0.51	0/407
32	1a	0.37	0/35795	0.88	22/55864 (0.0%)
32	2a	0.37	0/35886	0.89	21/56005 (0.0%)
33	1b	0.31	0/1881	0.51	0/2542
33	2b	0.31	0/1860	0.50	0/2518
34	1c	0.29	0/1572	0.46	0/2126
34	2c	0.30	0/1566	0.47	0/2119
35	1d	0.29	0/1685	0.49	0/2262
35	2d	0.30	0/1704	0.48	0/2284
36	1e	0.30	0/1145	0.51	0/1543
36	2e	0.31	0/1149	0.50	0/1548
37	1f	0.29	0/823	0.50	0/1115
37	2f	0.30	0/829	0.49	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.28	0/1250	0.42	0/1679
38	2g	0.29	0/1254	0.44	0/1683
39	1h	0.29	0/1108	0.47	0/1494
39	2h	0.30	0/1108	0.49	0/1494
40	1i	0.29	0/1002	0.47	0/1346
40	2i	0.31	0/997	0.49	1/1343 (0.1%)
41	1j	0.27	0/722	0.47	0/982
41	2j	0.30	0/727	0.49	0/988
42	1k	0.29	0/844	0.48	0/1145
42	2k	0.28	0/848	0.45	0/1149
43	1l	0.31	0/937	0.52	0/1260
43	2l	0.29	0/937	0.54	0/1260
44	1m	0.29	0/969	0.47	0/1302
44	2m	0.29	0/961	0.49	0/1291
45	1n	0.30	0/501	0.46	0/664
45	2n	0.31	0/501	0.47	0/664
46	1o	0.28	0/739	0.43	0/985
46	2o	0.27	0/739	0.46	0/985
47	1p	0.29	0/697	0.49	0/939
47	2p	0.28	0/693	0.47	0/935
48	1q	0.30	0/836	0.51	0/1117
48	2q	0.29	0/836	0.49	0/1117
49	1r	0.27	0/560	0.48	0/746
49	2r	0.29	0/560	0.52	0/746
50	1s	0.28	0/667	0.50	0/900
50	2s	0.29	0/661	0.58	1/893 (0.1%)
51	1t	0.28	0/730	0.50	1/965 (0.1%)
51	2t	0.28	0/729	0.42	0/965
52	1u	0.29	0/203	0.44	0/266
52	2u	0.28	0/203	0.49	0/266
53	1v	0.45	0/310	0.85	0/480
53	2v	0.52	0/310	0.91	0/480
54	1x	0.51	1/1725 (0.1%)	1.08	10/2689 (0.4%)
54	2x	0.45	0/1725	1.10	3/2689 (0.1%)
55	1z	0.34	0/153	0.56	0/207
55	2z	0.37	0/147	0.48	0/200
All	All	0.39	3/310535 (0.0%)	0.81	137/464519 (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
12	1Q	0	1
51	1t	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2B	1	U	OP3-P	-10.26	1.48	1.61
2	1B	1	U	OP3-P	-9.91	1.49	1.61
54	1x	14	A	C8-N7	-5.76	1.27	1.31

All (137) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2136	C	N1-C2-O2	11.38	125.73	118.90
1	1A	1075	C	N1-C2-O2	11.23	125.64	118.90
1	2A	1639	U	O5'-P-OP2	-8.72	97.85	105.70
1	2A	2139	C	C2-N1-C1'	8.42	128.06	118.80
1	1A	1075	C	N3-C2-O2	-8.31	116.09	121.90
1	1A	2167	U	C2-N1-C1'	8.28	127.63	117.70
1	1A	512	G	O4'-C1'-N9	7.88	114.50	108.20
1	2A	2136	C	N3-C2-O2	-7.64	116.55	121.90
54	1x	14	A	C5-N7-C8	7.62	107.71	103.90
32	1a	841	U	C2-N1-C1'	7.61	126.83	117.70
1	2A	2155	G	N3-C4-N9	7.61	130.56	126.00
32	1a	841	U	C5-C6-N1	7.60	126.50	122.70
1	2A	2155	G	C6-C5-N7	-7.55	125.87	130.40
2	2B	80	U	O4'-C1'-N1	7.52	114.21	108.20
32	2a	841	U	C5-C6-N1	7.51	126.46	122.70
32	1a	1030(B)	C	C2-N1-C1'	7.17	126.69	118.80
32	1a	1030(B)	C	N1-C2-O2	7.07	123.14	118.90
54	1x	22	G	N1-C6-O6	-7.04	115.67	119.90
1	1A	2167	U	N1-C2-O2	6.99	127.69	122.80
32	1a	1030(B)	C	C6-N1-C2	-6.98	117.51	120.30
1	2A	1532	C	C2-N1-C1'	6.89	126.38	118.80
1	2A	1993	U	O5'-P-OP1	-6.86	99.53	105.70
1	1A	2167	U	N3-C2-O2	-6.85	117.40	122.20
1	2A	2139	C	C6-N1-C1'	-6.76	112.69	120.80
1	2A	739	G	O5'-P-OP1	-6.74	99.64	105.70
1	1A	12	U	C2-N1-C1'	6.58	125.59	117.70
32	1a	1158	C	N1-C2-O2	6.50	122.80	118.90
1	2A	2155	G	C4-C5-N7	6.46	113.38	110.80
1	1A	1313	U	C2-N1-C1'	6.46	125.45	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1028	C	C2-N3-C4	6.41	123.10	119.90
32	1a	1158	C	C2-N1-C1'	6.41	125.84	118.80
1	2A	2155	G	N9-C4-C5	-6.39	102.84	105.40
32	1a	266	G	P-O3'-C3'	6.38	127.36	119.70
1	1A	2629	A	P-O3'-C3'	6.32	127.28	119.70
1	1A	1075	C	C2-N3-C4	6.30	123.05	119.90
32	2a	1126	U	C2-N1-C1'	6.29	125.25	117.70
1	2A	1532	C	N1-C2-O2	6.26	122.66	118.90
32	1a	1030(B)	C	N3-C2-O2	-6.18	117.57	121.90
6	2G	43	LEU	CA-CB-CG	6.16	129.46	115.30
54	1x	14	A	C4-C5-C6	6.14	120.07	117.00
1	2A	2689	U	P-O3'-C3'	6.13	127.05	119.70
1	2A	2152	G	C5-C6-O6	-6.07	124.96	128.60
1	1A	1063	G	C5-C6-O6	6.01	132.20	128.60
1	1A	1176	G	OP1-P-O3'	5.98	118.36	105.20
1	2A	1313	U	C2-N1-C1'	5.95	124.84	117.70
1	1A	1653	G	P-O3'-C3'	5.90	126.78	119.70
32	1a	841	U	N1-C2-O2	5.81	126.87	122.80
1	1A	1058	G	C5-C6-O6	5.79	132.08	128.60
32	2a	754	C	C2-N1-C1'	5.78	125.16	118.80
1	2A	2139	C	N1-C2-O2	5.77	122.36	118.90
32	1a	1002	G	N3-C4-N9	5.73	129.44	126.00
1	2A	2473	U	N1-C2-O2	5.69	126.78	122.80
32	2a	1037	C	C6-N1-C2	-5.68	118.03	120.30
1	2A	1992	G	C8-N9-C4	-5.67	104.13	106.40
1	1A	1992	G	P-O3'-C3'	5.65	126.48	119.70
54	2x	22	G	N1-C6-O6	-5.62	116.53	119.90
1	2A	2473	U	N3-C2-O2	-5.62	118.27	122.20
32	2a	1025	U	C2-N1-C1'	5.62	124.44	117.70
1	2A	1532	C	C6-N1-C1'	-5.62	114.06	120.80
32	2a	975	A	O4'-C1'-N9	-5.61	103.71	108.20
32	1a	841	U	C6-N1-C2	-5.60	117.64	121.00
1	1A	1979	C	C6-N1-C2	-5.56	118.08	120.30
32	1a	1067	A	P-O3'-C3'	5.55	126.36	119.70
54	1x	46	G	C6-N1-C2	-5.55	121.77	125.10
32	2a	979	C	C6-N1-C2	-5.55	118.08	120.30
32	2a	1025	U	N1-C2-O2	5.54	126.67	122.80
1	2A	2155	G	C4-N9-C1'	5.52	133.68	126.50
1	1A	115	C	O5'-P-OP1	-5.49	100.76	105.70
32	1a	563	A	O4'-C1'-N9	5.46	112.57	108.20
1	1A	975	C	N1-C2-O2	-5.42	115.65	118.90
32	2a	1186	G	N3-C2-N2	-5.42	116.11	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	266	G	N3-C4-C5	-5.38	125.91	128.60
1	2A	528	A	OP1-P-O3'	5.38	117.04	105.20
1	1A	2167	U	C5-C6-N1	5.38	125.39	122.70
1	2A	2473	U	C2-N1-C1'	5.37	124.14	117.70
54	1x	22	G	C5-C6-N1	5.36	114.18	111.50
1	1A	1074	G	C5-C6-O6	-5.36	125.39	128.60
54	1x	22	G	C6-C5-N7	5.35	133.61	130.40
1	1A	1075	C	C5-C4-N4	5.33	123.93	120.20
32	1a	1002	G	C4-N9-C1'	5.33	133.43	126.50
32	2a	1020	U	N1-C2-O2	5.33	126.53	122.80
32	2a	913	A	P-O3'-C3'	5.33	126.09	119.70
1	2A	1506	C	N1-C2-O2	5.31	122.09	118.90
1	1A	1174	A	P-O3'-C3'	5.30	126.06	119.70
1	1A	2407	G	C4-N9-C1'	5.30	133.39	126.50
54	1x	14	A	C4-C5-N7	-5.29	108.05	110.70
1	1A	652(S)	C	C2-N1-C1'	5.27	124.60	118.80
32	2a	754	C	N1-C2-O2	5.27	122.06	118.90
1	1A	1080	C	C2-N3-C4	5.26	122.53	119.90
1	1A	1313	U	N1-C2-O2	5.25	126.47	122.80
54	2x	14	A	C5-N7-C8	5.24	106.52	103.90
32	2a	1067	A	P-O3'-C3'	5.23	125.98	119.70
1	1A	530	G	OP1-P-O3'	5.23	116.70	105.20
1	1A	1063	G	N3-C2-N2	5.22	123.56	119.90
1	1A	801	G	O5'-P-OP2	-5.22	101.00	105.70
32	2a	1040	U	C5-C4-O4	-5.21	122.77	125.90
1	2A	1614	A	O5'-P-OP1	-5.21	101.01	105.70
32	2a	1212	U	C2-N1-C1'	5.21	123.95	117.70
32	1a	1158	C	N3-C2-O2	-5.20	118.26	121.90
1	2A	512	G	O4'-C1'-N9	5.20	112.36	108.20
54	2x	14	A	C4-C5-C6	5.17	119.59	117.00
32	1a	841	U	N3-C2-O2	-5.17	118.58	122.20
32	1a	687	A	P-O3'-C3'	5.17	125.90	119.70
32	1a	365	U	C2-N1-C1'	5.16	123.89	117.70
54	1x	22	G	C4-C5-C6	-5.16	115.70	118.80
54	1x	14	A	C8-N9-C1'	-5.16	118.42	127.70
32	1a	1054	C	C2-N1-C1'	5.16	124.47	118.80
1	2A	1210	A	P-O3'-C3'	5.16	125.89	119.70
32	2a	65	U	P-O3'-C3'	5.16	125.89	119.70
1	1A	1416	G	O4'-C1'-N9	5.16	112.32	108.20
51	1t	13	LEU	CA-CB-CG	5.16	127.16	115.30
1	1A	847	U	C2-N1-C1'	5.15	123.89	117.70
1	1A	1176	G	P-O3'-C3'	5.15	125.88	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1992	G	P-O3'-C3'	5.14	125.86	119.70
1	2A	2689	U	N3-C2-O2	-5.14	118.60	122.20
1	1A	2689	U	P-O3'-C3'	5.13	125.86	119.70
50	2s	16	LEU	CA-CB-CG	5.13	127.10	115.30
9	1N	106	MET	C-N-CA	5.12	134.50	121.70
1	2A	228	A	OP1-P-O3'	5.12	116.46	105.20
1	1A	1174	A	OP1-P-O3'	5.11	116.44	105.20
1	2A	1827	C	N1-C2-O2	5.10	121.96	118.90
1	2A	271(K)	U	C2-N1-C1'	5.10	123.82	117.70
1	1A	1063	G	C6-N1-C2	5.09	128.15	125.10
32	1a	1322	C	N1-C2-O2	-5.09	115.85	118.90
1	2A	2140	C	C6-N1-C2	-5.08	118.27	120.30
40	2i	102	LEU	CA-CB-CG	5.08	126.97	115.30
32	2a	1442	G	P-O3'-C3'	5.06	125.77	119.70
32	1a	913	A	P-O3'-C3'	5.04	125.74	119.70
1	2A	646	A	O4'-C1'-N9	5.04	112.23	108.20
1	1A	2167	U	C6-N1-C2	-5.03	117.98	121.00
1	1A	1046	A	O4'-C1'-N9	5.02	112.22	108.20
32	2a	99	U	N1-C2-O2	-5.02	119.29	122.80
32	2a	1033	G	C6-N1-C2	5.01	128.11	125.10
54	1x	14	A	C4-N9-C1'	5.01	135.31	126.30
1	1A	1314	C	C2-N1-C1'	5.00	124.31	118.80
1	1A	1394	U	O5'-P-OP1	-5.00	101.19	105.70
1	2A	2439	A	O4'-C1'-N9	-5.00	104.20	108.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	1Q	59	ARG	Peptide
51	1t	9	ASN	Peptide

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	252 (92%)	21 (8%)	0	100	100
3	2D	273/276 (99%)	245 (90%)	28 (10%)	0	100	100
4	1E	202/206 (98%)	188 (93%)	13 (6%)	1 (0%)	29	60
4	2E	202/206 (98%)	187 (93%)	13 (6%)	2 (1%)	15	45
5	1F	201/210 (96%)	190 (94%)	10 (5%)	1 (0%)	29	60
5	2F	201/210 (96%)	181 (90%)	17 (8%)	3 (2%)	10	35
6	1G	179/182 (98%)	161 (90%)	16 (9%)	2 (1%)	14	42
6	2G	179/182 (98%)	153 (86%)	22 (12%)	4 (2%)	6	25
7	1H	172/180 (96%)	154 (90%)	17 (10%)	1 (1%)	25	55
7	2H	172/180 (96%)	145 (84%)	25 (14%)	2 (1%)	13	40
8	1I	144/148 (97%)	123 (85%)	19 (13%)	2 (1%)	11	36
8	2I	144/148 (97%)	131 (91%)	10 (7%)	3 (2%)	7	26
9	1N	138/140 (99%)	130 (94%)	8 (6%)	0	100	100
9	2N	138/140 (99%)	123 (89%)	15 (11%)	0	100	100
10	1O	120/122 (98%)	108 (90%)	12 (10%)	0	100	100
10	2O	120/122 (98%)	103 (86%)	15 (12%)	2 (2%)	9	32
11	1P	147/150 (98%)	132 (90%)	15 (10%)	0	100	100
11	2P	147/150 (98%)	128 (87%)	16 (11%)	3 (2%)	7	27
12	1Q	139/141 (99%)	126 (91%)	10 (7%)	3 (2%)	6	25
12	2Q	139/141 (99%)	125 (90%)	14 (10%)	0	100	100
13	1R	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
13	2R	116/118 (98%)	104 (90%)	12 (10%)	0	100	100
14	1S	108/112 (96%)	102 (94%)	6 (6%)	0	100	100
14	2S	108/112 (96%)	95 (88%)	12 (11%)	1 (1%)	17	47
15	1T	129/146 (88%)	117 (91%)	12 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	2T	129/146 (88%)	119 (92%)	10 (8%)	0	100	100
16	1U	114/118 (97%)	112 (98%)	2 (2%)	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	45
17	2V	99/101 (98%)	87 (88%)	10 (10%)	2 (2%)	7	27
18	1W	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
18	2W	110/113 (97%)	105 (96%)	5 (4%)	0	100	100
19	1X	93/96 (97%)	86 (92%)	5 (5%)	2 (2%)	6	25
19	2X	93/96 (97%)	78 (84%)	15 (16%)	0	100	100
20	1Y	105/110 (96%)	92 (88%)	11 (10%)	2 (2%)	8	29
20	2Y	105/110 (96%)	90 (86%)	13 (12%)	2 (2%)	8	29
21	1Z	148/206 (72%)	128 (86%)	17 (12%)	3 (2%)	7	27
21	2Z	156/206 (76%)	130 (83%)	25 (16%)	1 (1%)	25	55
22	10	74/85 (87%)	72 (97%)	2 (3%)	0	100	100
22	20	74/85 (87%)	67 (90%)	6 (8%)	1 (1%)	11	36
23	11	95/98 (97%)	88 (93%)	6 (6%)	1 (1%)	14	42
23	21	95/98 (97%)	87 (92%)	8 (8%)	0	100	100
24	12	68/72 (94%)	63 (93%)	5 (7%)	0	100	100
24	22	68/72 (94%)	63 (93%)	5 (7%)	0	100	100
25	13	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
25	23	57/60 (95%)	50 (88%)	7 (12%)	0	100	100
26	14	67/71 (94%)	52 (78%)	10 (15%)	5 (8%)	1	4
26	24	67/71 (94%)	48 (72%)	14 (21%)	5 (8%)	1	4
27	15	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
27	25	57/60 (95%)	53 (93%)	3 (5%)	1 (2%)	8	30
28	16	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
28	26	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
29	17	46/49 (94%)	44 (96%)	2 (4%)	0	100	100
29	27	46/49 (94%)	43 (94%)	2 (4%)	1 (2%)	6	25
30	18	62/65 (95%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	59 (95%)	3 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	19	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
31	29	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
33	1b	229/256 (90%)	193 (84%)	25 (11%)	11 (5%)	2	11
33	2b	229/256 (90%)	185 (81%)	38 (17%)	6 (3%)	5	22
34	1c	204/239 (85%)	187 (92%)	16 (8%)	1 (0%)	29	60
34	2c	204/239 (85%)	166 (81%)	37 (18%)	1 (0%)	29	60
35	1d	206/209 (99%)	194 (94%)	11 (5%)	1 (0%)	29	60
35	2d	206/209 (99%)	178 (86%)	24 (12%)	4 (2%)	8	29
36	1e	146/162 (90%)	129 (88%)	15 (10%)	2 (1%)	11	36
36	2e	146/162 (90%)	127 (87%)	17 (12%)	2 (1%)	11	36
37	1f	98/101 (97%)	90 (92%)	7 (7%)	1 (1%)	15	45
37	2f	98/101 (97%)	88 (90%)	9 (9%)	1 (1%)	15	45
38	1g	153/156 (98%)	138 (90%)	10 (6%)	5 (3%)	4	17
38	2g	153/156 (98%)	131 (86%)	18 (12%)	4 (3%)	5	22
39	1h	135/138 (98%)	126 (93%)	8 (6%)	1 (1%)	22	52
39	2h	135/138 (98%)	120 (89%)	15 (11%)	0	100	100
40	1i	125/128 (98%)	110 (88%)	15 (12%)	0	100	100
40	2i	125/128 (98%)	109 (87%)	16 (13%)	0	100	100
41	1j	95/105 (90%)	81 (85%)	11 (12%)	3 (3%)	4	18
41	2j	94/105 (90%)	88 (94%)	5 (5%)	1 (1%)	14	42
42	1k	112/129 (87%)	99 (88%)	12 (11%)	1 (1%)	17	47
42	2k	112/129 (87%)	102 (91%)	7 (6%)	3 (3%)	5	21
43	1l	119/132 (90%)	111 (93%)	6 (5%)	2 (2%)	9	32
43	2l	119/132 (90%)	101 (85%)	16 (13%)	2 (2%)	9	32
44	1m	121/126 (96%)	105 (87%)	14 (12%)	2 (2%)	9	32
44	2m	120/126 (95%)	99 (82%)	18 (15%)	3 (2%)	5	22
45	1n	58/61 (95%)	55 (95%)	2 (3%)	1 (2%)	9	32
45	2n	58/61 (95%)	51 (88%)	5 (9%)	2 (3%)	3	17
46	1o	86/89 (97%)	76 (88%)	8 (9%)	2 (2%)	6	24
46	2o	86/89 (97%)	80 (93%)	6 (7%)	0	100	100
47	1p	80/88 (91%)	67 (84%)	13 (16%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	2p	80/88 (91%)	71 (89%)	8 (10%)	1 (1%)	12	38
48	1q	97/105 (92%)	84 (87%)	11 (11%)	2 (2%)	7	26
48	2q	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
49	1r	66/88 (75%)	59 (89%)	7 (11%)	0	100	100
49	2r	66/88 (75%)	62 (94%)	4 (6%)	0	100	100
50	1s	81/93 (87%)	69 (85%)	10 (12%)	2 (2%)	5	22
50	2s	81/93 (87%)	68 (84%)	12 (15%)	1 (1%)	13	40
51	1t	94/106 (89%)	84 (89%)	8 (8%)	2 (2%)	7	26
51	2t	94/106 (89%)	83 (88%)	8 (8%)	3 (3%)	4	18
52	1u	21/27 (78%)	18 (86%)	3 (14%)	0	100	100
52	2u	21/27 (78%)	15 (71%)	4 (19%)	2 (10%)	0	3
55	1z	14/16 (88%)	12 (86%)	1 (7%)	1 (7%)	1	5
55	2z	14/16 (88%)	13 (93%)	1 (7%)	0	100	100
All	All	11384/12160 (94%)	10190 (90%)	1061 (9%)	133 (1%)	13	40

All (133) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
6	1G	43	LEU
7	1H	126	PRO
12	1Q	24	GLY
12	1Q	60	ARG
21	1Z	93	ASP
26	14	45	GLY
33	1b	22	LYS
33	1b	126	GLU
35	1d	5	ILE
38	1g	4	ARG
38	1g	80	VAL
41	1j	79	ARG
44	1m	67	GLU
44	1m	106	ASN
50	1s	81	ARG
5	2F	130	ALA
33	2b	16	HIS
33	2b	17	PHE

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Mol	Chain	Res	Type
36	2e	98	THR
38	2g	80	VAL
38	2g	114	ARG
44	2m	67	GLU
52	2u	3	LYS
8	1I	42	SER
19	1X	93	GLU
23	1I	3	LYS
26	14	50	VAL
26	14	61	ARG
33	1b	13	ALA
33	1b	17	PHE
33	1b	129	GLU
34	1c	107	GLN
36	1e	85	GLY
38	1g	6	ARG
38	1g	55	GLY
43	1I	104	VAL
43	1I	106	ASP
45	1n	19	ARG
6	2G	51	ARG
8	2I	10	GLU
10	2O	54	GLU
11	2P	36	LYS
26	24	45	GLY
38	2g	7	ALA
38	2g	55	GLY
42	2k	49	GLY
44	2m	106	ASN
51	2t	47	GLY
4	1E	52	LEU
12	1Q	59	ARG
17	1V	79	VAL
20	1Y	54	LYS
21	1Z	120	ILE
26	14	62	ARG
33	1b	20	GLU
48	1q	67	LYS
8	2I	106	GLY
14	2S	96	GLY
22	20	33	ALA
36	2e	77	PRO

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Mol	Chain	Res	Type
41	2j	78	ASN
51	2t	99	LEU
33	1b	124	SER
33	1b	125	PRO
33	1b	231	GLU
38	1g	86	GLN
46	1o	86	GLY
46	1o	88	ARG
51	1t	10	LEU
51	1t	47	GLY
55	1z	15	TRP
4	2E	52	LEU
4	2E	157	ALA
5	2F	166	ALA
6	2G	44	GLY
6	2G	48	GLU
6	2G	170	ARG
8	2I	117	GLU
17	2V	79	VAL
20	2Y	80	GLY
26	24	29	PRO
26	24	49	PHE
35	2d	48	ALA
35	2d	167	GLY
37	2f	38	GLU
50	2s	54	GLY
52	2u	4	GLY
6	1G	110	ALA
8	1I	117	GLU
33	1b	202	PRO
33	1b	234	PRO
37	1f	38	GLU
41	1j	26	ALA
42	1k	49	GLY
48	1q	68	ARG
50	1s	24	ALA
5	2F	188	ARG
7	2H	69	ARG
10	2O	5	GLN
11	2P	28	GLY
17	2V	53	GLU
20	2Y	51	VAL

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Mol	Chain	Res	Type
21	2Z	90	VAL
26	24	19	GLY
26	24	48	ARG
27	25	57	VAL
33	2b	10	LEU
33	2b	78	GLN
42	2k	106	LYS
43	2l	91	LYS
45	2n	52	GLN
51	2t	95	ALA
20	1Y	103	GLY
41	1j	39	PRO
33	2b	20	GLU
35	2d	73	ARG
43	2l	104	VAL
45	2n	27	CYS
21	1Z	134	PRO
39	1h	83	ILE
33	2b	125	PRO
26	14	29	PRO
7	2H	29	PRO
44	2m	6	GLY
19	1X	94	GLY
11	2P	23	PRO
29	27	46	VAL
34	2c	55	VAL
35	2d	136	PRO
36	1e	69	VAL
42	2k	76	GLY
47	2p	53	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%)	190 (88%)	25 (12%)	5 19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	2D	215/218 (99%)	192 (89%)	23 (11%)	6	23
4	1E	164/166 (99%)	146 (89%)	18 (11%)	6	22
4	2E	164/166 (99%)	146 (89%)	18 (11%)	6	22
5	1F	160/166 (96%)	146 (91%)	14 (9%)	10	32
5	2F	159/166 (96%)	140 (88%)	19 (12%)	5	18
6	1G	143/156 (92%)	130 (91%)	13 (9%)	9	30
6	2G	143/156 (92%)	122 (85%)	21 (15%)	3	11
7	1H	144/148 (97%)	128 (89%)	16 (11%)	6	21
7	2H	144/148 (97%)	137 (95%)	7 (5%)	25	55
8	1I	113/124 (91%)	101 (89%)	12 (11%)	6	23
8	2I	105/124 (85%)	91 (87%)	14 (13%)	4	14
9	1N	118/119 (99%)	107 (91%)	11 (9%)	9	29
9	2N	118/119 (99%)	105 (89%)	13 (11%)	6	22
10	1O	100/100 (100%)	95 (95%)	5 (5%)	24	54
10	2O	100/100 (100%)	97 (97%)	3 (3%)	41	69
11	1P	115/116 (99%)	103 (90%)	12 (10%)	7	24
11	2P	115/116 (99%)	102 (89%)	13 (11%)	6	21
12	1Q	111/111 (100%)	103 (93%)	8 (7%)	14	40
12	2Q	111/111 (100%)	95 (86%)	16 (14%)	3	12
13	1R	101/101 (100%)	93 (92%)	8 (8%)	12	36
13	2R	101/101 (100%)	97 (96%)	4 (4%)	31	62
14	1S	86/88 (98%)	73 (85%)	13 (15%)	3	10
14	2S	85/88 (97%)	73 (86%)	12 (14%)	3	13
15	1T	115/127 (91%)	107 (93%)	8 (7%)	15	41
15	2T	113/127 (89%)	101 (89%)	12 (11%)	6	23
16	1U	93/94 (99%)	89 (96%)	4 (4%)	29	59
16	2U	93/94 (99%)	91 (98%)	2 (2%)	52	76
17	1V	80/82 (98%)	72 (90%)	8 (10%)	7	25
17	2V	80/82 (98%)	72 (90%)	8 (10%)	7	25
18	1W	90/92 (98%)	83 (92%)	7 (8%)	12	37
18	2W	90/92 (98%)	84 (93%)	6 (7%)	16	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	1X	77/78 (99%)	75 (97%)	2 (3%)	46	72
19	2X	77/78 (99%)	75 (97%)	2 (3%)	46	72
20	1Y	85/91 (93%)	78 (92%)	7 (8%)	11	35
20	2Y	85/91 (93%)	80 (94%)	5 (6%)	19	47
21	1Z	135/179 (75%)	123 (91%)	12 (9%)	9	31
21	2Z	137/179 (76%)	120 (88%)	17 (12%)	4	17
22	10	61/67 (91%)	56 (92%)	5 (8%)	11	35
22	20	61/67 (91%)	57 (93%)	4 (7%)	16	43
23	11	80/83 (96%)	74 (92%)	6 (8%)	13	39
23	21	80/83 (96%)	73 (91%)	7 (9%)	10	32
24	12	65/67 (97%)	58 (89%)	7 (11%)	6	22
24	22	65/67 (97%)	61 (94%)	4 (6%)	18	46
25	13	51/52 (98%)	45 (88%)	6 (12%)	5	18
25	23	50/52 (96%)	45 (90%)	5 (10%)	7	25
26	14	59/63 (94%)	53 (90%)	6 (10%)	7	24
26	24	53/63 (84%)	44 (83%)	9 (17%)	2	8
27	15	50/52 (96%)	44 (88%)	6 (12%)	5	18
27	25	50/52 (96%)	46 (92%)	4 (8%)	12	36
28	16	51/52 (98%)	46 (90%)	5 (10%)	8	26
28	26	50/52 (96%)	42 (84%)	8 (16%)	2	9
29	17	41/42 (98%)	37 (90%)	4 (10%)	8	26
29	27	41/42 (98%)	38 (93%)	3 (7%)	14	40
30	18	54/55 (98%)	50 (93%)	4 (7%)	13	39
30	28	54/55 (98%)	51 (94%)	3 (6%)	21	49
31	19	34/34 (100%)	33 (97%)	1 (3%)	42	70
31	29	34/34 (100%)	31 (91%)	3 (9%)	10	32
33	1b	192/220 (87%)	172 (90%)	20 (10%)	7	24
33	2b	187/220 (85%)	170 (91%)	17 (9%)	9	30
34	1c	142/188 (76%)	123 (87%)	19 (13%)	4	14
34	2c	140/188 (74%)	119 (85%)	21 (15%)	3	11
35	1d	169/181 (93%)	147 (87%)	22 (13%)	4	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	2d	173/181 (96%)	160 (92%)	13 (8%)	13	39
36	1e	113/123 (92%)	104 (92%)	9 (8%)	12	36
36	2e	114/123 (93%)	100 (88%)	14 (12%)	4	17
37	1f	84/90 (93%)	78 (93%)	6 (7%)	14	41
37	2f	85/90 (94%)	78 (92%)	7 (8%)	11	35
38	1g	119/127 (94%)	107 (90%)	12 (10%)	7	25
38	2g	120/127 (94%)	108 (90%)	12 (10%)	7	25
39	1h	114/119 (96%)	102 (90%)	12 (10%)	7	23
39	2h	114/119 (96%)	105 (92%)	9 (8%)	12	36
40	1i	90/99 (91%)	82 (91%)	8 (9%)	9	31
40	2i	89/99 (90%)	79 (89%)	10 (11%)	6	21
41	1j	66/92 (72%)	62 (94%)	4 (6%)	18	46
41	2j	69/92 (75%)	58 (84%)	11 (16%)	2	9
42	1k	82/99 (83%)	75 (92%)	7 (8%)	10	34
42	2k	83/99 (84%)	75 (90%)	8 (10%)	8	27
43	1l	96/108 (89%)	82 (85%)	14 (15%)	3	12
43	2l	96/108 (89%)	86 (90%)	10 (10%)	7	24
44	1m	93/101 (92%)	79 (85%)	14 (15%)	3	10
44	2m	92/101 (91%)	81 (88%)	11 (12%)	5	18
45	1n	49/50 (98%)	42 (86%)	7 (14%)	3	12
45	2n	49/50 (98%)	43 (88%)	6 (12%)	5	17
46	1o	78/80 (98%)	73 (94%)	5 (6%)	17	44
46	2o	78/80 (98%)	72 (92%)	6 (8%)	13	38
47	1p	69/74 (93%)	57 (83%)	12 (17%)	2	7
47	2p	68/74 (92%)	60 (88%)	8 (12%)	5	18
48	1q	94/97 (97%)	85 (90%)	9 (10%)	8	27
48	2q	94/97 (97%)	89 (95%)	5 (5%)	22	51
49	1r	59/77 (77%)	56 (95%)	3 (5%)	24	53
49	2r	59/77 (77%)	53 (90%)	6 (10%)	7	24
50	1s	69/80 (86%)	65 (94%)	4 (6%)	20	48
50	2s	67/80 (84%)	56 (84%)	11 (16%)	2	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	1t	70/82 (85%)	62 (89%)	8 (11%)	5	20
51	2t	70/82 (85%)	67 (96%)	3 (4%)	29	59
52	1u	18/22 (82%)	17 (94%)	1 (6%)	21	49
52	2u	18/22 (82%)	16 (89%)	2 (11%)	6	21
55	1z	15/16 (94%)	13 (87%)	2 (13%)	4	14
55	2z	14/16 (88%)	13 (93%)	1 (7%)	14	41
All	All	9324/10096 (92%)	8417 (90%)	907 (10%)	8	27

All (907) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	3	VAL
3	1D	12	SER
3	1D	14	ARG
3	1D	22	SER
3	1D	32	SER
3	1D	53	PHE
3	1D	61	LEU
3	1D	66	ASP
3	1D	88	ARG
3	1D	99	ASP
3	1D	106	ILE
3	1D	122	ASP
3	1D	140	THR
3	1D	141	VAL
3	1D	142	VAL
3	1D	193	VAL
3	1D	200	ASP
3	1D	211	ARG
3	1D	217	ARG
3	1D	221	VAL
3	1D	229	VAL
3	1D	242	ARG
3	1D	254	THR
3	1D	266	SER
3	1D	273	ARG
4	1E	5	LEU
4	1E	7	VAL
4	1E	9	VAL
4	1E	12	THR

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Mol	Chain	Res	Type
4	1E	21	VAL
4	1E	23	VAL
4	1E	24	THR
4	1E	34	VAL
4	1E	41	LYS
4	1E	75	VAL
4	1E	82	ARG
4	1E	93	VAL
4	1E	97	LYS
4	1E	116	VAL
4	1E	149	ARG
4	1E	152	LYS
4	1E	170	LEU
4	1E	178	GLU
5	1F	52	LYS
5	1F	53	THR
5	1F	57	VAL
5	1F	64	ILE
5	1F	74	ARG
5	1F	88	VAL
5	1F	106	ARG
5	1F	153	SER
5	1F	158	THR
5	1F	175	THR
5	1F	183	VAL
5	1F	189	THR
5	1F	195	ASP
5	1F	201	VAL
6	1G	5	VAL
6	1G	21	ARG
6	1G	28	VAL
6	1G	49	ASP
6	1G	91	ARG
6	1G	128	ARG
6	1G	138	GLN
6	1G	139	LEU
6	1G	145	THR
6	1G	150	ASP
6	1G	159	VAL
6	1G	161	THR
6	1G	162	THR
7	1H	2	SER

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Mol	Chain	Res	Type
7	1H	15	VAL
7	1H	16	SER
7	1H	18	GLU
7	1H	45	VAL
7	1H	47	GLU
7	1H	49	VAL
7	1H	68	THR
7	1H	72	ILE
7	1H	98	LEU
7	1H	99	VAL
7	1H	105	LEU
7	1H	119	GLU
7	1H	122	THR
7	1H	136	ILE
7	1H	155	SER
8	1I	10	GLU
8	1I	47	LEU
8	1I	57	ARG
8	1I	74	ASN
8	1I	82	ARG
8	1I	87	LYS
8	1I	92	VAL
8	1I	93	THR
8	1I	96	ASP
8	1I	109	ILE
8	1I	140	LEU
8	1I	145	VAL
9	1N	22	THR
9	1N	28	THR
9	1N	33	LEU
9	1N	34	LEU
9	1N	46	VAL
9	1N	48	MET
9	1N	62	VAL
9	1N	73	THR
9	1N	88	GLU
9	1N	99	LEU
9	1N	120	LEU
10	1O	10	VAL
10	1O	24	VAL
10	1O	53	LYS
10	1O	69	ILE

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Mol	Chain	Res	Type
10	1O	78	ARG
11	1P	3	LEU
11	1P	29	LYS
11	1P	30	THR
11	1P	42	SER
11	1P	56	SER
11	1P	59	LEU
11	1P	65	ARG
11	1P	67	MET
11	1P	95	VAL
11	1P	98	GLU
11	1P	117	GLU
11	1P	125	VAL
12	1Q	7	MET
12	1Q	35	VAL
12	1Q	56	ARG
12	1Q	59	ARG
12	1Q	75	THR
12	1Q	85	LYS
12	1Q	110	THR
12	1Q	113	GLN
13	1R	1	MET
13	1R	6	SER
13	1R	8	ARG
13	1R	15	SER
13	1R	33	ARG
13	1R	44	LEU
13	1R	59	ASP
13	1R	111	LEU
14	1S	12	PHE
14	1S	14	VAL
14	1S	17	ARG
14	1S	36	TYR
14	1S	46	VAL
14	1S	50	SER
14	1S	52	SER
14	1S	68	GLN
14	1S	69	VAL
14	1S	80	LEU
14	1S	85	VAL
14	1S	89	ARG
14	1S	98	VAL

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Mol	Chain	Res	Type
15	1T	9	LEU
15	1T	28	VAL
15	1T	29	ARG
15	1T	74	ARG
15	1T	89	VAL
15	1T	96	ARG
15	1T	118	ARG
15	1T	128	GLU
16	1U	8	VAL
16	1U	74	LEU
16	1U	83	LEU
16	1U	101	ARG
17	1V	7	THR
17	1V	46	VAL
17	1V	52	VAL
17	1V	61	VAL
17	1V	72	VAL
17	1V	73	SER
17	1V	79	VAL
17	1V	82	ARG
18	1W	23	LEU
18	1W	37	ARG
18	1W	60	ASN
18	1W	90	ARG
18	1W	92	ARG
18	1W	101	SER
18	1W	109	GLU
19	1X	23	GLU
19	1X	95	LEU
20	1Y	1	MET
20	1Y	7	VAL
20	1Y	9	LYS
20	1Y	55	TYR
20	1Y	70	SER
20	1Y	72	VAL
20	1Y	92	ASN
21	1Z	5	LEU
21	1Z	24	LEU
21	1Z	31	ARG
21	1Z	56	VAL
21	1Z	72	ARG
21	1Z	73	GLN

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Mol	Chain	Res	Type
21	1Z	80	ARG
21	1Z	84	GLU
21	1Z	87	ASP
21	1Z	123	ASP
21	1Z	129	SER
21	1Z	136	PHE
22	10	10	THR
22	10	11	ARG
22	10	14	ARG
22	10	53	MET
22	10	68	GLU
23	11	30	VAL
23	11	41	ARG
23	11	51	VAL
23	11	59	THR
23	11	83	GLU
23	11	95	LEU
24	12	1	MET
24	12	3	LEU
24	12	19	VAL
24	12	40	SER
24	12	52	ASP
24	12	53	LEU
24	12	60	LEU
25	13	31	LEU
25	13	40	THR
25	13	56	VAL
25	13	58	VAL
25	13	59	VAL
25	13	60	GLU
26	14	22	ILE
26	14	48	ARG
26	14	49	PHE
26	14	56	VAL
26	14	59	PHE
26	14	63	TYR
27	15	6	VAL
27	15	15	ARG
27	15	16	ARG
27	15	26	THR
27	15	40	LYS
27	15	55	ARG

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Mol	Chain	Res	Type
28	16	5	VAL
28	16	6	ARG
28	16	13	CYS
28	16	19	ARG
28	16	48	VAL
29	17	1	MET
29	17	24	THR
29	17	41	ARG
29	17	46	VAL
30	18	14	VAL
30	18	23	VAL
30	18	31	HIS
30	18	34	TRP
31	19	1	MET
33	1b	8	LYS
33	1b	10	LEU
33	1b	19	HIS
33	1b	21	ARG
33	1b	24	TRP
33	1b	30	ARG
33	1b	69	LEU
33	1b	81	VAL
33	1b	95	GLN
33	1b	112	VAL
33	1b	117	GLU
33	1b	122	PHE
33	1b	140	HIS
33	1b	160	ASP
33	1b	164	VAL
33	1b	172	ILE
33	1b	185	ILE
33	1b	217	ARG
33	1b	226	ARG
33	1b	230	VAL
34	1c	15	THR
34	1c	28	GLN
34	1c	36	ASP
34	1c	45	LYS
34	1c	52	LEU
34	1c	59	ARG
34	1c	64	VAL
34	1c	70	VAL

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Mol	Chain	Res	Type
34	1c	77	ILE
34	1c	85	ARG
34	1c	105	GLU
34	1c	111	LEU
34	1c	119	ARG
34	1c	124	ILE
34	1c	154	SER
34	1c	166	GLU
34	1c	172	ARG
34	1c	195	VAL
34	1c	204	LEU
35	1d	3	ARG
35	1d	5	ILE
35	1d	8	VAL
35	1d	10	ARG
35	1d	12	CYS
35	1d	45	GLN
35	1d	51	PRO
35	1d	59	ARG
35	1d	65	ARG
35	1d	86	LYS
35	1d	91	SER
35	1d	93	PHE
35	1d	123	HIS
35	1d	127	THR
35	1d	135	LEU
35	1d	157	LEU
35	1d	158	ILE
35	1d	186	LEU
35	1d	190	ASP
35	1d	194	LEU
35	1d	196	LEU
35	1d	208	SER
36	1e	10	MET
36	1e	16	THR
36	1e	27	ARG
36	1e	40	ARG
36	1e	41	VAL
36	1e	67	VAL
36	1e	79	GLU
36	1e	88	LYS
36	1e	91	LEU

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Mol	Chain	Res	Type
37	1f	21	LEU
37	1f	55	ASP
37	1f	64	GLN
37	1f	73	ASN
37	1f	75	LEU
37	1f	91	VAL
38	1g	13	GLN
38	1g	15	ASP
38	1g	28	ASN
38	1g	38	LEU
38	1g	45	ASP
38	1g	47	CYS
38	1g	72	ARG
38	1g	80	VAL
38	1g	113	GLU
38	1g	115	ARG
38	1g	135	VAL
38	1g	140	ASP
39	1h	3	THR
39	1h	18	ARG
39	1h	19	VAL
39	1h	49	GLU
39	1h	59	LEU
39	1h	63	LEU
39	1h	85	ARG
39	1h	104	ARG
39	1h	109	ILE
39	1h	112	LEU
39	1h	115	SER
39	1h	122	ARG
40	1i	53	VAL
40	1i	86	VAL
40	1i	92	TYR
40	1i	103	THR
40	1i	104	ARG
40	1i	121	ARG
40	1i	127	LYS
40	1i	128	ARG
41	1j	38	ILE
41	1j	46	ARG
41	1j	67	THR
41	1j	84	GLN

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Mol	Chain	Res	Type
42	1k	48	ILE
42	1k	50	TYR
42	1k	57	THR
42	1k	81	ASP
42	1k	87	THR
42	1k	114	VAL
42	1k	116	HIS
43	1l	18	VAL
43	1l	33	ARG
43	1l	36	VAL
43	1l	40	VAL
43	1l	42	THR
43	1l	54	LYS
43	1l	55	VAL
43	1l	66	VAL
43	1l	78	GLN
43	1l	83	VAL
43	1l	91	LYS
43	1l	105	TYR
43	1l	118	SER
43	1l	123	LYS
44	1m	4	ILE
44	1m	8	GLU
44	1m	11	ARG
44	1m	34	LEU
44	1m	43	THR
44	1m	49	THR
44	1m	63	THR
44	1m	64	TRP
44	1m	94	ARG
44	1m	105	THR
44	1m	106	ASN
44	1m	109	THR
44	1m	114	ARG
44	1m	116	THR
45	1n	7	ILE
45	1n	17	LYS
45	1n	18	VAL
45	1n	22	THR
45	1n	29	ARG
45	1n	33	VAL
45	1n	60	SER

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Mol	Chain	Res	Type
46	1o	5	LYS
46	1o	7	GLU
46	1o	21	ASP
46	1o	56	LEU
46	1o	77	ARG
47	1p	1	MET
47	1p	2	VAL
47	1p	6	LEU
47	1p	11	SER
47	1p	35	LYS
47	1p	38	TYR
47	1p	42	ARG
47	1p	45	THR
47	1p	54	GLU
47	1p	62	VAL
47	1p	67	THR
47	1p	72	ARG
48	1q	19	VAL
48	1q	52	LYS
48	1q	60	ILE
48	1q	63	ARG
48	1q	69	LYS
48	1q	74	LEU
48	1q	87	LYS
48	1q	93	GLN
48	1q	96	GLU
49	1r	23	LYS
49	1r	66	LEU
49	1r	82	THR
50	1s	12	ASP
50	1s	30	LEU
50	1s	48	THR
50	1s	49	ILE
51	1t	9	ASN
51	1t	10	LEU
51	1t	51	GLU
51	1t	55	ILE
51	1t	75	ASN
51	1t	80	ARG
51	1t	91	LEU
51	1t	100	ILE
52	1u	15	ARG

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Mol	Chain	Res	Type
55	1z	9	ARG
55	1z	14	ARG
3	2D	3	VAL
3	2D	38	LYS
3	2D	54	ARG
3	2D	69	ARG
3	2D	94	LEU
3	2D	99	ASP
3	2D	106	ILE
3	2D	111	LEU
3	2D	113	VAL
3	2D	131	LEU
3	2D	134	ARG
3	2D	138	VAL
3	2D	142	VAL
3	2D	157	ARG
3	2D	183	ARG
3	2D	200	ASP
3	2D	211	ARG
3	2D	221	VAL
3	2D	229	VAL
3	2D	237	GLU
3	2D	242	ARG
3	2D	267	SER
3	2D	276	LYS
4	2E	1	MET
4	2E	9	VAL
4	2E	17	ASP
4	2E	21	VAL
4	2E	24	THR
4	2E	33	VAL
4	2E	52	LEU
4	2E	75	VAL
4	2E	90	THR
4	2E	91	VAL
4	2E	94	GLU
4	2E	102	VAL
4	2E	116	VAL
4	2E	156	MET
4	2E	173	VAL
4	2E	181	LEU
4	2E	184	VAL

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Mol	Chain	Res	Type
4	2E	195	LEU
5	2F	12	LEU
5	2F	33	LEU
5	2F	46	ARG
5	2F	51	THR
5	2F	65	TRP
5	2F	74	ARG
5	2F	88	VAL
5	2F	108	LYS
5	2F	110	LEU
5	2F	127	GLU
5	2F	132	VAL
5	2F	135	LYS
5	2F	153	SER
5	2F	183	VAL
5	2F	192	LEU
5	2F	197	ASP
5	2F	200	GLU
5	2F	201	VAL
5	2F	206	ILE
6	2G	5	VAL
6	2G	9	ARG
6	2G	10	LYS
6	2G	21	ARG
6	2G	28	VAL
6	2G	43	LEU
6	2G	47	LYS
6	2G	51	ARG
6	2G	60	LEU
6	2G	96	ARG
6	2G	108	ASN
6	2G	130	ASN
6	2G	133	LEU
6	2G	135	LEU
6	2G	140	ILE
6	2G	145	THR
6	2G	152	LEU
6	2G	159	VAL
6	2G	161	THR
6	2G	165	THR
6	2G	170	ARG
7	2H	35	VAL

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Mol	Chain	Res	Type
7	2H	50	VAL
7	2H	99	VAL
7	2H	106	THR
7	2H	119	GLU
7	2H	124	GLU
7	2H	131	VAL
8	2I	12	LEU
8	2I	20	ASP
8	2I	31	LEU
8	2I	38	LEU
8	2I	44	LEU
8	2I	51	ILE
8	2I	75	LEU
8	2I	85	GLU
8	2I	92	VAL
8	2I	93	THR
8	2I	101	LEU
8	2I	107	VAL
8	2I	140	LEU
8	2I	144	VAL
9	2N	12	ARG
9	2N	21	LYS
9	2N	22	THR
9	2N	28	THR
9	2N	33	LEU
9	2N	34	LEU
9	2N	43	THR
9	2N	48	MET
9	2N	60	ILE
9	2N	74	ARG
9	2N	96	GLU
9	2N	98	VAL
9	2N	127	ASP
10	2O	9	GLU
10	2O	96	THR
10	2O	97	ARG
11	2P	32	THR
11	2P	36	LYS
11	2P	42	SER
11	2P	45	LEU
11	2P	56	SER
11	2P	57	THR

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Mol	Chain	Res	Type
11	2P	75	ILE
11	2P	86	LYS
11	2P	94	GLU
11	2P	95	VAL
11	2P	100	LEU
11	2P	138	LEU
11	2P	148	LEU
12	2Q	1	MET
12	2Q	21	THR
12	2Q	25	ASP
12	2Q	38	GLU
12	2Q	55	VAL
12	2Q	65	PHE
12	2Q	79	LEU
12	2Q	85	LYS
12	2Q	90	VAL
12	2Q	106	VAL
12	2Q	109	VAL
12	2Q	110	THR
12	2Q	112	GLU
12	2Q	129	THR
12	2Q	133	ARG
12	2Q	135	ASP
13	2R	11	ASN
13	2R	28	LEU
13	2R	29	LEU
13	2R	107	ASP
14	2S	5	THR
14	2S	8	GLU
14	2S	13	ARG
14	2S	17	ARG
14	2S	21	THR
14	2S	27	SER
14	2S	48	LEU
14	2S	52	SER
14	2S	58	LEU
14	2S	75	GLU
14	2S	78	LEU
14	2S	98	VAL
15	2T	15	VAL
15	2T	28	VAL
15	2T	38	ASN

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Mol	Chain	Res	Type
15	2T	39	ARG
15	2T	49	VAL
15	2T	51	ARG
15	2T	63	VAL
15	2T	64	ARG
15	2T	89	VAL
15	2T	96	ARG
15	2T	107	ASP
15	2T	108	ARG
16	2U	31	SER
16	2U	74	LEU
17	2V	13	ARG
17	2V	14	VAL
17	2V	38	LEU
17	2V	46	VAL
17	2V	70	ILE
17	2V	79	VAL
17	2V	82	ARG
17	2V	93	GLU
18	2W	17	VAL
18	2W	67	ASP
18	2W	70	TYR
18	2W	100	THR
18	2W	107	LEU
18	2W	109	GLU
19	2X	43	VAL
19	2X	45	THR
20	2Y	6	HIS
20	2Y	7	VAL
20	2Y	19	LYS
20	2Y	38	ILE
20	2Y	71	LYS
21	2Z	33	LEU
21	2Z	42	VAL
21	2Z	46	LYS
21	2Z	66	SER
21	2Z	69	THR
21	2Z	71	VAL
21	2Z	86	VAL
21	2Z	93	ASP
21	2Z	94	GLU
21	2Z	121	HIS

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Mol	Chain	Res	Type
21	2Z	123	ASP
21	2Z	126	VAL
21	2Z	144	LEU
21	2Z	154	ASP
21	2Z	161	VAL
21	2Z	171	ILE
21	2Z	174	VAL
22	20	11	ARG
22	20	14	ARG
22	20	64	ASP
22	20	74	ARG
23	21	4	VAL
23	21	14	VAL
23	21	35	THR
23	21	59	THR
23	21	61	ARG
23	21	65	SER
23	21	95	LEU
24	22	10	LEU
24	22	40	SER
24	22	53	LEU
24	22	70	GLN
25	23	5	LYS
25	23	30	ARG
25	23	32	GLN
25	23	52	HIS
25	23	53	LEU
26	24	5	ILE
26	24	10	VAL
26	24	34	GLU
26	24	42	PHE
26	24	44	THR
26	24	49	PHE
26	24	50	VAL
26	24	56	VAL
26	24	63	TYR
27	25	6	VAL
27	25	16	ARG
27	25	29	THR
27	25	56	LYS
28	26	6	ARG
28	26	15	GLU

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Mol	Chain	Res	Type
28	26	32	ASN
28	26	40	CYS
28	26	48	VAL
28	26	49	HIS
28	26	51	GLU
28	26	54	ILE
29	27	10	ARG
29	27	42	LEU
29	27	48	LYS
30	28	14	VAL
30	28	31	HIS
30	28	32	LEU
31	29	6	SER
31	29	7	VAL
31	29	22	ARG
33	2b	8	LYS
33	2b	24	TRP
33	2b	33	TYR
33	2b	40	HIS
33	2b	44	LEU
33	2b	83	MET
33	2b	93	VAL
33	2b	107	THR
33	2b	119	GLU
33	2b	127	ILE
33	2b	160	ASP
33	2b	168	THR
33	2b	187	LEU
33	2b	195	ASP
33	2b	220	ASP
33	2b	224	GLN
33	2b	230	VAL
34	2c	15	THR
34	2c	30	ARG
34	2c	32	LEU
34	2c	34	LEU
34	2c	48	TYR
34	2c	54	ARG
34	2c	55	VAL
34	2c	63	ASN
34	2c	67	THR
34	2c	77	ILE

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Mol	Chain	Res	Type
34	2c	98	ASN
34	2c	125	GLU
34	2c	151	VAL
34	2c	153	VAL
34	2c	157	ILE
34	2c	164	ARG
34	2c	178	LEU
34	2c	179	ARG
34	2c	186	PHE
34	2c	190	ARG
34	2c	191	THR
35	2d	31	CYS
35	2d	76	ARG
35	2d	78	LEU
35	2d	94	LEU
35	2d	96	LEU
35	2d	108	LEU
35	2d	118	ARG
35	2d	135	LEU
35	2d	138	TYR
35	2d	141	ARG
35	2d	144	ASP
35	2d	170	VAL
35	2d	194	LEU
36	2e	10	MET
36	2e	18	ARG
36	2e	27	ARG
36	2e	37	ARG
36	2e	41	VAL
36	2e	53	LEU
36	2e	55	VAL
36	2e	78	HIS
36	2e	81	GLU
36	2e	87	SER
36	2e	120	THR
36	2e	133	TYR
36	2e	144	THR
36	2e	150	ARG
37	2f	10	LEU
37	2f	17	SER
37	2f	19	LEU
37	2f	37	VAL

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Mol	Chain	Res	Type
37	2f	40	VAL
37	2f	78	GLU
37	2f	89	MET
38	2g	6	ARG
38	2g	9	VAL
38	2g	16	LEU
38	2g	22	LEU
38	2g	56	GLN
38	2g	73	MET
38	2g	76	ARG
38	2g	79	ARG
38	2g	91	VAL
38	2g	102	ARG
38	2g	105	VAL
38	2g	115	ARG
39	2h	8	ASP
39	2h	32	LYS
39	2h	37	ARG
39	2h	46	LYS
39	2h	52	ASP
39	2h	60	ARG
39	2h	99	GLU
39	2h	104	ARG
39	2h	109	ILE
40	2i	27	THR
40	2i	56	LEU
40	2i	60	ASP
40	2i	75	ASP
40	2i	102	LEU
40	2i	105	ASP
40	2i	108	VAL
40	2i	117	HIS
40	2i	121	ARG
40	2i	124	GLN
41	2j	13	HIS
41	2j	15	THR
41	2j	21	GLN
41	2j	29	ARG
41	2j	34	VAL
41	2j	65	LEU
41	2j	67	THR
41	2j	72	VAL

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Mol	Chain	Res	Type
41	2j	73	ASP
41	2j	85	LEU
41	2j	95	GLU
42	2k	14	VAL
42	2k	28	THR
42	2k	50	TYR
42	2k	66	LEU
42	2k	93	GLN
42	2k	101	SER
42	2k	107	SER
42	2k	114	VAL
43	2l	33	ARG
43	2l	40	VAL
43	2l	52	LEU
43	2l	57	LYS
43	2l	66	VAL
43	2l	86	ARG
43	2l	89	ARG
43	2l	102	ARG
43	2l	105	TYR
43	2l	117	ARG
44	2m	8	GLU
44	2m	19	LEU
44	2m	47	ASP
44	2m	48	LEU
44	2m	55	ARG
44	2m	64	TRP
44	2m	74	VAL
44	2m	78	ILE
44	2m	91	ARG
44	2m	93	ARG
44	2m	103	THR
45	2n	3	ARG
45	2n	11	LYS
45	2n	13	THR
45	2n	18	VAL
45	2n	33	VAL
45	2n	44	LEU
46	2o	6	GLU
46	2o	54	ARG
46	2o	56	LEU
46	2o	59	MET

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Mol	Chain	Res	Type
46	2o	72	ARG
46	2o	76	GLU
47	2p	2	VAL
47	2p	6	LEU
47	2p	20	VAL
47	2p	21	VAL
47	2p	40	ASP
47	2p	45	THR
47	2p	49	LEU
47	2p	69	THR
48	2q	7	THR
48	2q	15	MET
48	2q	62	SER
48	2q	74	LEU
48	2q	86	GLU
49	2r	38	GLU
49	2r	44	LEU
49	2r	45	SER
49	2r	54	ARG
49	2r	84	LYS
49	2r	85	LEU
50	2s	3	ARG
50	2s	14	HIS
50	2s	16	LEU
50	2s	30	LEU
50	2s	33	THR
50	2s	37	ARG
50	2s	41	VAL
50	2s	65	ASN
50	2s	66	MET
50	2s	79	THR
50	2s	83	HIS
51	2t	10	LEU
51	2t	56	MET
51	2t	70	SER
52	2u	3	LYS
52	2u	15	ARG
55	2z	4	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (125) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	87	ASN
3	1D	201	HIS
3	1D	220	HIS
4	1E	48	GLN
4	1E	143	ASN
4	1E	180	ASN
5	1F	8	GLN
5	1F	67	GLN
5	1F	203	GLN
6	1G	132	ASN
6	1G	138	GLN
8	1I	54	GLN
8	1I	139	GLN
10	1O	3	GLN
11	1P	84	ASN
12	1Q	57	HIS
13	1R	91	GLN
15	1T	58	ASN
16	1U	117	GLN
18	1W	60	ASN
19	1X	31	HIS
21	1Z	32	HIS
21	1Z	151	HIS
24	12	46	GLN
26	14	60	GLN
31	19	29	ASN
33	1b	16	HIS
33	1b	40	HIS
34	1c	6	HIS
34	1c	28	GLN
34	1c	162	GLN
34	1c	170	GLN
35	1d	42	GLN
35	1d	116	GLN
35	1d	119	GLN
35	1d	123	HIS
35	1d	160	GLN
36	1e	20	GLN
36	1e	78	HIS
37	1f	7	ASN
37	1f	13	ASN
37	1f	73	ASN
37	1f	100	ASN

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Mol	Chain	Res	Type
38	1g	13	GLN
38	1g	28	ASN
38	1g	97	GLN
39	1h	82	HIS
40	1i	3	GLN
40	1i	29	ASN
40	1i	31	GLN
40	1i	34	ASN
40	1i	38	GLN
40	1i	58	HIS
40	1i	124	GLN
41	1j	56	HIS
42	1k	93	GLN
44	1m	106	ASN
46	1o	13	GLN
47	1p	13	HIS
47	1p	65	GLN
48	1q	45	HIS
49	1r	63	GLN
50	1s	57	HIS
50	1s	83	HIS
3	2D	87	ASN
3	2D	126	GLN
3	2D	253	GLN
4	2E	48	GLN
4	2E	66	HIS
5	2F	133	ASN
6	2G	26	GLN
6	2G	130	ASN
8	2I	139	GLN
10	2O	90	GLN
11	2P	27	HIS
12	2Q	12	GLN
12	2Q	89	ASN
13	2R	11	ASN
13	2R	24	GLN
13	2R	91	GLN
14	2S	38	GLN
15	2T	55	ASN
15	2T	58	ASN
15	2T	123	GLN
16	2U	117	GLN

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Mol	Chain	Res	Type
17	2V	64	HIS
17	2V	80	GLN
21	2Z	32	HIS
21	2Z	34	ASN
21	2Z	55	HIS
21	2Z	73	GLN
21	2Z	75	ASN
23	21	19	GLN
23	21	56	GLN
24	22	65	ASN
25	23	32	GLN
26	24	46	GLN
27	25	23	HIS
28	26	20	ASN
29	27	6	GLN
33	2b	40	HIS
34	2c	6	HIS
34	2c	37	GLN
34	2c	102	ASN
34	2c	162	GLN
35	2d	116	GLN
35	2d	123	HIS
35	2d	161	ASN
35	2d	201	GLN
36	2e	56	GLN
36	2e	65	ASN
37	2f	100	ASN
40	2i	38	GLN
40	2i	73	GLN
41	2j	21	GLN
42	2k	38	ASN
42	2k	117	ASN
44	2m	12	ASN
44	2m	77	ASN
49	2r	63	GLN
50	2s	14	HIS
50	2s	23	ASN
51	2t	9	ASN
51	2t	42	GLN
51	2t	75	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2860/2915 (98%)	472 (16%)	26 (0%)
1	2A	2788/2915 (95%)	508 (18%)	22 (0%)
2	1B	119/121 (98%)	11 (9%)	0
2	2B	118/121 (97%)	32 (27%)	0
32	1a	1494/1521 (98%)	263 (17%)	0
32	2a	1498/1521 (98%)	304 (20%)	0
53	1v	12/24 (50%)	5 (41%)	0
53	2v	12/24 (50%)	5 (41%)	0
54	1x	75/77 (97%)	9 (12%)	0
54	2x	75/77 (97%)	11 (14%)	0
All	All	9051/9316 (97%)	1620 (17%)	48 (0%)

All (1620) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	13	A
1	1A	34	C
1	1A	45	C
1	1A	50	U
1	1A	55	G
1	1A	61	G
1	1A	63	U
1	1A	64	A
1	1A	71	A
1	1A	74	A
1	1A	75	G
1	1A	84	A
1	1A	102	G
1	1A	118	A
1	1A	119	A
1	1A	120	U
1	1A	125	G
1	1A	141	A
1	1A	177	G
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	225	A

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Mol	Chain	Res	Type
1	1A	228	A
1	1A	229	A
1	1A	230	U
1	1A	233	A
1	1A	241	A
1	1A	248	G
1	1A	269	U
1	1A	271(L)	U
1	1A	271(M)	G
1	1A	271(O)	C
1	1A	271(P)	C
1	1A	272(B)	G
1	1A	279	C
1	1A	294	A
1	1A	308	G
1	1A	311	A
1	1A	324	A
1	1A	329	G
1	1A	330	A
1	1A	342	G
1	1A	352	G
1	1A	363	G
1	1A	363(B)	G
1	1A	371	A
1	1A	372	G
1	1A	383	U
1	1A	386	G
1	1A	396	G
1	1A	405	U
1	1A	407	G
1	1A	411	G
1	1A	412	A
1	1A	428	A
1	1A	444	C
1	1A	448	U
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	508	G

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Mol	Chain	Res	Type
1	1A	509	C
1	1A	530	G
1	1A	531	C
1	1A	532	A
1	1A	533	G
1	1A	549	G
1	1A	563	G
1	1A	573	G
1	1A	574	C
1	1A	575	A
1	1A	603	A
1	1A	604	G
1	1A	607	U
1	1A	610	G
1	1A	614(A)	U
1	1A	614(B)	G
1	1A	614(C)	A
1	1A	615	G
1	1A	619	G
1	1A	627	A
1	1A	631	A
1	1A	637	A
1	1A	645	C
1	1A	646	A
1	1A	648	G
1	1A	652(E)	G
1	1A	652(T)	C
1	1A	669	G
1	1A	686	G
1	1A	717	G
1	1A	719	C
1	1A	730	C
1	1A	740	U
1	1A	764	A
1	1A	775	G
1	1A	776	G
1	1A	782	A
1	1A	784	A
1	1A	785	G
1	1A	789	A
1	1A	792	G
1	1A	793	A

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Mol	Chain	Res	Type
1	1A	794	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	831	G
1	1A	869	G
1	1A	879	G
1	1A	880	G
1	1A	881	G
1	1A	884	C
1	1A	885	C
1	1A	886	C
1	1A	887	A
1	1A	888	C
1	1A	889	C
1	1A	890	A
1	1A	896	A
1	1A	897	C
1	1A	898	C
1	1A	910	A
1	1A	932	G
1	1A	938	G
1	1A	945	A
1	1A	946	G
1	1A	953	A
1	1A	959	A
1	1A	961	C
1	1A	968	G
1	1A	974	G
1	1A	975	C
1	1A	975(A)	G
1	1A	983	A
1	1A	996	A
1	1A	1012	U
1	1A	1013	C
1	1A	1022	G
1	1A	1026	U
1	1A	1027	A
1	1A	1033	U

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Mol	Chain	Res	Type
1	1A	1038	C
1	1A	1041	C
1	1A	1044	G
1	1A	1045	A
1	1A	1046	A
1	1A	1047	G
1	1A	1054	A
1	1A	1055	G
1	1A	1057	A
1	1A	1058	G
1	1A	1059	G
1	1A	1064	C
1	1A	1066	U
1	1A	1068	G
1	1A	1070	A
1	1A	1071	G
1	1A	1073	A
1	1A	1074	G
1	1A	1075	C
1	1A	1076	C
1	1A	1078	U
1	1A	1079	C
1	1A	1081	U
1	1A	1088	A
1	1A	1094	U
1	1A	1096	A
1	1A	1101	U
1	1A	1105	U
1	1A	1110	G
1	1A	1112	G
1	1A	1116	C
1	1A	1129	A
1	1A	1130	U
1	1A	1135	C
1	1A	1136	G
1	1A	1141	U
1	1A	1142(A)	A
1	1A	1155	A
1	1A	1170	G
1	1A	1171	G
1	1A	1173	G
1	1A	1174	A

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Mol	Chain	Res	Type
1	1A	1175	U
1	1A	1176	G
1	1A	1177	A
1	1A	1189	A
1	1A	1218	C
1	1A	1250	G
1	1A	1253	A
1	1A	1256	G
1	1A	1268	A
1	1A	1271	G
1	1A	1272	A
1	1A	1273	U
1	1A	1274	A
1	1A	1275	A
1	1A	1287	A
1	1A	1300	U
1	1A	1301	A
1	1A	1320	C
1	1A	1329	U
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	1395	A
1	1A	1396	U
1	1A	1416	G
1	1A	1417	C
1	1A	1420	U
1	1A	1421	G
1	1A	1428	C
1	1A	1437	C
1	1A	1445	A
1	1A	1450	G
1	1A	1453	U
1	1A	1455	G
1	1A	1461	G
1	1A	1467	C

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Mol	Chain	Res	Type
1	1A	1482	G
1	1A	1493	C
1	1A	1497	U
1	1A	1507	A
1	1A	1509	C
1	1A	1509(A)	A
1	1A	1525	G
1	1A	1540	U
1	1A	1542	A
1	1A	1543	C
1	1A	1558	A
1	1A	1566	A
1	1A	1569	A
1	1A	1578	U
1	1A	1581	G
1	1A	1584	C
1	1A	1586	A
1	1A	1608	A
1	1A	1609	A
1	1A	1610	A
1	1A	1616	A
1	1A	1646	C
1	1A	1647	G
1	1A	1648	C
1	1A	1654	A
1	1A	1667	G
1	1A	1674	G
1	1A	1676	A
1	1A	1700	A
1	1A	1701	A
1	1A	1722	A
1	1A	1739	U
1	1A	1746	G
1	1A	1762	A
1	1A	1763	G
1	1A	1764	G
1	1A	1773	A
1	1A	1780	A
1	1A	1781	C
1	1A	1782	C
1	1A	1791	A
1	1A	1800	C

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Mol	Chain	Res	Type
1	1A	1816	G
1	1A	1829	A
1	1A	1847	A
1	1A	1858	G
1	1A	1878	G
1	1A	1900	A
1	1A	1906	G
1	1A	1913	A
1	1A	1914	C
1	1A	1919	A
1	1A	1927	A
1	1A	1929	G
1	1A	1930	G
1	1A	1934	C
1	1A	1936	A
1	1A	1937	A
1	1A	1938	A
1	1A	1941	C
1	1A	1952	A
1	1A	1955	U
1	1A	1963	U
1	1A	1965	C
1	1A	1967	C
1	1A	1970	A
1	1A	1971	A
1	1A	1972	A
1	1A	1992	G
1	1A	1993	U
1	1A	1997	G
1	1A	2020	A
1	1A	2021	C
1	1A	2023	G
1	1A	2027	G
1	1A	2031	A
1	1A	2032	G
1	1A	2033	A
1	1A	2039	C
1	1A	2043	C
1	1A	2055	C
1	1A	2056	G
1	1A	2060	A
1	1A	2061	G

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Mol	Chain	Res	Type
1	1A	2062	A
1	1A	2067	G
1	1A	2069	G
1	1A	2096	U
1	1A	2097	C
1	1A	2099	U
1	1A	2101	G
1	1A	2110	G
1	1A	2112	G
1	1A	2113	U
1	1A	2114	A
1	1A	2121	G
1	1A	2123	G
1	1A	2125	G
1	1A	2126	A
1	1A	2127	G
1	1A	2129	C
1	1A	2131	G
1	1A	2132	U
1	1A	2133	G
1	1A	2134	A
1	1A	2135	A
1	1A	2140	C
1	1A	2142	C
1	1A	2144	U
1	1A	2146	C
1	1A	2149	G
1	1A	2151	G
1	1A	2152	G
1	1A	2156	G
1	1A	2157	G
1	1A	2158	A
1	1A	2159	G
1	1A	2161	C
1	1A	2163	C
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	2175	C

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Mol	Chain	Res	Type
1	1A	2178	C
1	1A	2181	G
1	1A	2182	G
1	1A	2183	C
1	1A	2184	G
1	1A	2192	G
1	1A	2198	A
1	1A	2206	G
1	1A	2207	G
1	1A	2208	A
1	1A	2219	G
1	1A	2225	A
1	1A	2238	G
1	1A	2239	G
1	1A	2267	A
1	1A	2268	A
1	1A	2269	A
1	1A	2283	C
1	1A	2287	A
1	1A	2294	C
1	1A	2295	C
1	1A	2305	A
1	1A	2308	G
1	1A	2309	A
1	1A	2312	U
1	1A	2315	G
1	1A	2320	A
1	1A	2325	G
1	1A	2334	G
1	1A	2336	A
1	1A	2347	C
1	1A	2350	C
1	1A	2361	A
1	1A	2372	G
1	1A	2377	A
1	1A	2383	G
1	1A	2385	C
1	1A	2391	G
1	1A	2406	U
1	1A	2425	A
1	1A	2429	G
1	1A	2430	A

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Mol	Chain	Res	Type
1	1A	2432	A
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	2498	C
1	1A	2502	G
1	1A	2505	G
1	1A	2506	U
1	1A	2518	A
1	1A	2520	C
1	1A	2529	G
1	1A	2549	G
1	1A	2554	U
1	1A	2566	A
1	1A	2567	G
1	1A	2570	G
1	1A	2582	G
1	1A	2586	C
1	1A	2602	A
1	1A	2604	U
1	1A	2609	U
1	1A	2611	U
1	1A	2612	C
1	1A	2615	U
1	1A	2629	A
1	1A	2630	G
1	1A	2654	A
1	1A	2663	G
1	1A	2670	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
1	1A	2713	A
1	1A	2726	U
1	1A	2733	A
1	1A	2739	U

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Mol	Chain	Res	Type
1	1A	2744	G
1	1A	2757	A
1	1A	2761	G
1	1A	2765	A
1	1A	2766	G
1	1A	2769	C
1	1A	2778	A
1	1A	2790	A
1	1A	2791	C
1	1A	2792	G
1	1A	2802	G
1	1A	2803	C
1	1A	2807	G
1	1A	2808	U
1	1A	2818	G
1	1A	2820	A
1	1A	2821	A
1	1A	2833	G
1	1A	2835	A
1	1A	2850	A
1	1A	2872	G
1	1A	2880	C
1	1A	2892	A
1	1A	2894	G
2	1B	2	C
2	1B	10	C
2	1B	12	C
2	1B	13	A
2	1B	33	G
2	1B	42	C
2	1B	56	G
2	1B	73	A
2	1B	98	G
2	1B	106	G
2	1B	110	G
32	1a	7	G
32	1a	9	G
32	1a	10	A
32	1a	22	G
32	1a	32	A
32	1a	39	G
32	1a	47	C

Continued on next page...

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Mol	Chain	Res	Type
32	1a	48	C
32	1a	50	A
32	1a	51	A
32	1a	54	C
32	1a	61	G
32	1a	69	G
32	1a	73	G
32	1a	79	G
32	1a	91	C
32	1a	98	G
32	1a	101	A
32	1a	111	G
32	1a	116	A
32	1a	121	C
32	1a	122	G
32	1a	129(A)	G
32	1a	131	C
32	1a	140	A
32	1a	144	G
32	1a	145	G
32	1a	146	G
32	1a	162	A
32	1a	163	C
32	1a	164	U
32	1a	174	C
32	1a	182	U
32	1a	189(D)	C
32	1a	189(G)	G
32	1a	189(H)	G
32	1a	189(L)	G
32	1a	195	A
32	1a	197	A
32	1a	201	C
32	1a	202	U
32	1a	203	U
32	1a	204	U
32	1a	216	G
32	1a	222	U
32	1a	247	G
32	1a	251	G
32	1a	266	G
32	1a	267	C

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Mol	Chain	Res	Type
32	1a	274	A
32	1a	289	G
32	1a	301	G
32	1a	321	A
32	1a	328	C
32	1a	332	G
32	1a	342	C
32	1a	344	A
32	1a	348	G
32	1a	351	G
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	356	A
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	384	G
32	1a	397	A
32	1a	398	C
32	1a	406	G
32	1a	412	A
32	1a	413	G
32	1a	424	G
32	1a	428	G
32	1a	429	U
32	1a	439	A
32	1a	452	A
32	1a	453	A
32	1a	461	A
32	1a	470	C
32	1a	475	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	531	U
32	1a	532	A

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Mol	Chain	Res	Type
32	1a	533	A
32	1a	547	A
32	1a	559	A
32	1a	560	U
32	1a	561	U
32	1a	562	C
32	1a	564	C
32	1a	568	G
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	577	G
32	1a	581	G
32	1a	596	C
32	1a	607	A
32	1a	610	G
32	1a	622	A
32	1a	630	G
32	1a	653	A
32	1a	657	G
32	1a	665	A
32	1a	671	G
32	1a	687	A
32	1a	688	G
32	1a	695	A
32	1a	717	C
32	1a	721	G
32	1a	724	G
32	1a	731	G
32	1a	749	C
32	1a	755	G
32	1a	759	A
32	1a	777	A
32	1a	787	A
32	1a	792	A
32	1a	793	U
32	1a	794	A
32	1a	816	A
32	1a	817	C
32	1a	821	G
32	1a	828	A
32	1a	840	C

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Mol	Chain	Res	Type
32	1a	841	U
32	1a	851	G
32	1a	852	G
32	1a	856	C
32	1a	859	A
32	1a	872	A
32	1a	876	G
32	1a	885	G
32	1a	889	A
32	1a	902	G
32	1a	909	A
32	1a	914	A
32	1a	926	G
32	1a	927	G
32	1a	934	C
32	1a	935	A
32	1a	936	C
32	1a	939	G
32	1a	940	C
32	1a	960	U
32	1a	961	U
32	1a	963	G
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	974	A
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	992	U
32	1a	993	G
32	1a	997	U
32	1a	1000	U
32	1a	1002	G
32	1a	1003	G
32	1a	1005	A
32	1a	1006	C
32	1a	1008	C
32	1a	1009	G
32	1a	1022	G
32	1a	1024	G
32	1a	1025	U

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Mol	Chain	Res	Type
32	1a	1026	G
32	1a	1027	C
32	1a	1028	C
32	1a	1029	C
32	1a	1030(A)	G
32	1a	1030(C)	G
32	1a	1031	G
32	1a	1034	G
32	1a	1036	G
32	1a	1037	C
32	1a	1044	A
32	1a	1053	G
32	1a	1054	C
32	1a	1065	U
32	1a	1066	C
32	1a	1068	G
32	1a	1081	G
32	1a	1086	U
32	1a	1094	G
32	1a	1096	C
32	1a	1101	A
32	1a	1124	G
32	1a	1125	U
32	1a	1126	U
32	1a	1131	G
32	1a	1132	C
32	1a	1134	G
32	1a	1136	U
32	1a	1137	C
32	1a	1138	G
32	1a	1139	G
32	1a	1152	A
32	1a	1157	A
32	1a	1159	U
32	1a	1179	A
32	1a	1184	G
32	1a	1196	U
32	1a	1197	G
32	1a	1202	G
32	1a	1212	U
32	1a	1213	A
32	1a	1214	C

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Mol	Chain	Res	Type
32	1a	1227	A
32	1a	1236	A
32	1a	1238	A
32	1a	1256	A
32	1a	1257	U
32	1a	1264	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	1298	C
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1320	C
32	1a	1340	A
32	1a	1346	A
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1397	C
32	1a	1400	5MC
32	1a	1401	G
32	1a	1419	G
32	1a	1436	U
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1446	U
32	1a	1447	A
32	1a	1456	G
32	1a	1492	A
32	1a	1493	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

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Mol	Chain	Res	Type
32	1a	1520	G
32	1a	1529	G
32	1a	1530	G
32	1a	1532	U
53	1v	13	A
53	1v	15	A
53	1v	19	U
53	1v	20	U
53	1v	24	A
54	1x	6	G
54	1x	9	G
54	1x	14	A
54	1x	18	G
54	1x	20	U
54	1x	21	A
54	1x	47	U
54	1x	67	C
54	1x	76	A
1	2A	12	U
1	2A	14	A
1	2A	15	G
1	2A	34	C
1	2A	35	G
1	2A	45	C
1	2A	51	G
1	2A	57	C
1	2A	60	G
1	2A	63	U
1	2A	64	A
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	78	A
1	2A	79	G
1	2A	84	A
1	2A	90	U
1	2A	100	G
1	2A	102	G
1	2A	112	U
1	2A	118	A
1	2A	120	U
1	2A	140	G

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Mol	Chain	Res	Type
1	2A	154(A)	C
1	2A	157	U
1	2A	181	A
1	2A	196	A
1	2A	199	A
1	2A	205	G
1	2A	214	G
1	2A	216	A
1	2A	221	A
1	2A	222	A
1	2A	227	A
1	2A	228	A
1	2A	229	A
1	2A	233	A
1	2A	248	G
1	2A	249	C
1	2A	250	G
1	2A	266	G
1	2A	271(H)	G
1	2A	271(K)	U
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	271(O)	C
1	2A	271(T)	C
1	2A	272(B)	G
1	2A	277	C
1	2A	278	A
1	2A	279	C
1	2A	284	U
1	2A	294	A
1	2A	299	A
1	2A	302	C
1	2A	311	A
1	2A	316	C
1	2A	317	G
1	2A	324	A
1	2A	327	G
1	2A	329	G
1	2A	330	A
1	2A	352	G
1	2A	362	U

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Mol	Chain	Res	Type
1	2A	363	G
1	2A	363(B)	G
1	2A	386	G
1	2A	396	G
1	2A	404	C
1	2A	405	U
1	2A	407	G
1	2A	411	G
1	2A	412	A
1	2A	422	A
1	2A	425	G
1	2A	444	C
1	2A	454	A
1	2A	455	C
1	2A	480	A
1	2A	481	G
1	2A	482	A
1	2A	496	G
1	2A	501	A
1	2A	504	U
1	2A	505	A
1	2A	509	C
1	2A	527	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	551	G
1	2A	556	G
1	2A	563	G
1	2A	568	U
1	2A	573	G
1	2A	575	A
1	2A	599	G
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	614(B)	G
1	2A	615	G
1	2A	627	A

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Mol	Chain	Res	Type
1	2A	637	A
1	2A	645	C
1	2A	651	G
1	2A	652(B)	A
1	2A	652(C)	G
1	2A	653	A
1	2A	669	G
1	2A	677	A
1	2A	686	G
1	2A	730	C
1	2A	753	C
1	2A	764	A
1	2A	775	G
1	2A	776	G
1	2A	779	U
1	2A	782	A
1	2A	784	A
1	2A	785	G
1	2A	805	G
1	2A	809	G
1	2A	812	C
1	2A	819	A
1	2A	825	C
1	2A	827	U
1	2A	828	U
1	2A	830	G
1	2A	843	G
1	2A	847	U
1	2A	857	C
1	2A	859	G
1	2A	869	G
1	2A	874	G
1	2A	879	G
1	2A	880	G
1	2A	882	G
1	2A	883	G
1	2A	884	C
1	2A	886	C
1	2A	887	A
1	2A	888	C
1	2A	889	C
1	2A	892	G

Continued on next page...

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Mol	Chain	Res	Type
1	2A	893	C
1	2A	894	C
1	2A	895	U
1	2A	896	A
1	2A	897	C
1	2A	898	C
1	2A	900	A
1	2A	901	A
1	2A	904	C
1	2A	907	U
1	2A	910	A
1	2A	914	C
1	2A	917	A
1	2A	931	G
1	2A	932	G
1	2A	933	A
1	2A	941	A
1	2A	945	A
1	2A	946	G
1	2A	953	A
1	2A	958	U
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	1003	G
1	2A	1012	U
1	2A	1013	C
1	2A	1017	G
1	2A	1022	G
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	1042	G
1	2A	1043	C
1	2A	1114	G
1	2A	1116	C

Continued on next page...

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Mol	Chain	Res	Type
1	2A	1127	A
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1142	U
1	2A	1142(A)	A
1	2A	1144	G
1	2A	1164	G
1	2A	1171	G
1	2A	1206	G
1	2A	1210	A
1	2A	1211	U
1	2A	1220	A
1	2A	1229	G
1	2A	1236	G
1	2A	1237	A
1	2A	1248	G
1	2A	1253	A
1	2A	1255	U
1	2A	1256	G
1	2A	1257	C
1	2A	1271	G
1	2A	1272	A
1	2A	1273	U
1	2A	1300	U
1	2A	1301	A
1	2A	1314	C
1	2A	1327	C
1	2A	1341	U
1	2A	1345	C
1	2A	1352	U
1	2A	1359	A
1	2A	1360	A
1	2A	1365	A
1	2A	1370	C
1	2A	1379	A
1	2A	1383	C
1	2A	1384	A
1	2A	1385	G
1	2A	1386	C
1	2A	1416	G
1	2A	1417	C

Continued on next page...

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Mol	Chain	Res	Type
1	2A	1419	A
1	2A	1421	G
1	2A	1427	A
1	2A	1428	C
1	2A	1437	C
1	2A	1447	G
1	2A	1448	G
1	2A	1449	A
1	2A	1450	G
1	2A	1455	G
1	2A	1460	A
1	2A	1467	C
1	2A	1471	A
1	2A	1477	A
1	2A	1482	G
1	2A	1490	A
1	2A	1493	C
1	2A	1494	A
1	2A	1495	A
1	2A	1496	A
1	2A	1497	U
1	2A	1504	C
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1531	C
1	2A	1542	A
1	2A	1543	C
1	2A	1547	C
1	2A	1558	A
1	2A	1559	G
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1580	A
1	2A	1584	C
1	2A	1586	A
1	2A	1594	G
1	2A	1602	U
1	2A	1603	A
1	2A	1608	A
1	2A	1609	A

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Mol	Chain	Res	Type
1	2A	1610	A
1	2A	1634	A
1	2A	1640	C
1	2A	1647	G
1	2A	1648	C
1	2A	1654	A
1	2A	1671	U
1	2A	1674	G
1	2A	1680	U
1	2A	1682	G
1	2A	1694	C
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	1739	U
1	2A	1740	G
1	2A	1745	C
1	2A	1746	G
1	2A	1756	G
1	2A	1758	G
1	2A	1762	A
1	2A	1763	G
1	2A	1764	G
1	2A	1773	A
1	2A	1780	A
1	2A	1782	C
1	2A	1786	A
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1812	A
1	2A	1816	G
1	2A	1827	C
1	2A	1828	G
1	2A	1829	A
1	2A	1835	G
1	2A	1836	C
1	2A	1847	A
1	2A	1848	A

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Mol	Chain	Res	Type
1	2A	1877	A
1	2A	1878	G
1	2A	1889	A
1	2A	1900	A
1	2A	1906	G
1	2A	1913	A
1	2A	1914	C
1	2A	1927	A
1	2A	1929	G
1	2A	1930	G
1	2A	1936	A
1	2A	1937	A
1	2A	1938	A
1	2A	1955	U
1	2A	1963	U
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1993	U
1	2A	1997	G
1	2A	2021	C
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	2066	C
1	2A	2069	G
1	2A	2099	U
1	2A	2104	G
1	2A	2107	C
1	2A	2111	C
1	2A	2112	G
1	2A	2113	U
1	2A	2115	G
1	2A	2116	G

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Mol	Chain	Res	Type
1	2A	2117	A
1	2A	2120	G
1	2A	2126	A
1	2A	2127	G
1	2A	2129	C
1	2A	2131	G
1	2A	2132	U
1	2A	2133	G
1	2A	2134	A
1	2A	2135	A
1	2A	2136	C
1	2A	2137	C
1	2A	2138	C
1	2A	2140	C
1	2A	2142	C
1	2A	2144	U
1	2A	2146	C
1	2A	2148	G
1	2A	2150	U
1	2A	2153	G
1	2A	2155	G
1	2A	2156	G
1	2A	2157	G
1	2A	2158	A
1	2A	2161	C
1	2A	2164	C
1	2A	2166	G
1	2A	2167	U
1	2A	2168	G
1	2A	2169	A
1	2A	2172	U
1	2A	2178	C
1	2A	2182	G
1	2A	2185	C
1	2A	2188	C
1	2A	2192	G
1	2A	2197	U
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2218	U

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Mol	Chain	Res	Type
1	2A	2219	G
1	2A	2225	A
1	2A	2235	G
1	2A	2238	G
1	2A	2239	G
1	2A	2243	U
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	2305	A
1	2A	2307	G
1	2A	2308	G
1	2A	2309	A
1	2A	2319	G
1	2A	2320	A
1	2A	2325	G
1	2A	2334	G
1	2A	2336	A
1	2A	2345	G
1	2A	2347	C
1	2A	2350	C
1	2A	2354	G
1	2A	2366	A
1	2A	2383	G
1	2A	2385	C
1	2A	2406	U
1	2A	2425	A
1	2A	2428	G
1	2A	2429	G
1	2A	2430	A
1	2A	2434	A
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2448	A
1	2A	2459	A
1	2A	2469	A
1	2A	2474	C
1	2A	2476	A

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Mol	Chain	Res	Type
1	2A	2477	C
1	2A	2490	G
1	2A	2502	G
1	2A	2504	U
1	2A	2505	G
1	2A	2506	U
1	2A	2518	A
1	2A	2527	C
1	2A	2529	G
1	2A	2549	G
1	2A	2554	U
1	2A	2564	A
1	2A	2566	A
1	2A	2567	G
1	2A	2582	G
1	2A	2585	U
1	2A	2586	C
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	2641	G
1	2A	2654	A
1	2A	2667	C
1	2A	2689	U
1	2A	2690	C
1	2A	2703	C
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G
1	2A	2726	U
1	2A	2730	C
1	2A	2733	A
1	2A	2744	G
1	2A	2748	A
1	2A	2751	G
1	2A	2752	C
1	2A	2757	A
1	2A	2758	A
1	2A	2764	A

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Mol	Chain	Res	Type
1	2A	2765	A
1	2A	2766	G
1	2A	2778	A
1	2A	2789	C
1	2A	2802	G
1	2A	2803	C
1	2A	2804	C
1	2A	2808	U
1	2A	2810	A
1	2A	2818	G
1	2A	2820	A
1	2A	2821	A
1	2A	2833	G
1	2A	2835	A
1	2A	2858	C
1	2A	2872	G
1	2A	2873	A
1	2A	2876	G
1	2A	2879	C
1	2A	2880	C
1	2A	2894	G
1	2A	2897	U
2	2B	2	C
2	2B	5	C
2	2B	8	U
2	2B	9	G
2	2B	12	C
2	2B	13	A
2	2B	15	A
2	2B	21	G
2	2B	24	G
2	2B	25	A
2	2B	30	C
2	2B	42	C
2	2B	52	A
2	2B	53	A
2	2B	55	U
2	2B	56	G
2	2B	58	A
2	2B	60	C
2	2B	63	G
2	2B	67	G

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Mol	Chain	Res	Type
2	2B	71	C
2	2B	72	G
2	2B	73	A
2	2B	74	U
2	2B	75	G
2	2B	85	G
2	2B	108	U
2	2B	110	G
2	2B	111	G
2	2B	114	C
2	2B	116	G
2	2B	120	A
32	2a	6	G
32	2a	7	G
32	2a	9	G
32	2a	22	G
32	2a	32	A
32	2a	39	G
32	2a	44	G
32	2a	47	C
32	2a	48	C
32	2a	50	A
32	2a	51	A
32	2a	66	G
32	2a	72	C
32	2a	73	G
32	2a	78	G
32	2a	89	C
32	2a	91	C
32	2a	101	A
32	2a	116	A
32	2a	121	C
32	2a	129(A)	G
32	2a	131	C
32	2a	142	G
32	2a	143	A
32	2a	144	G
32	2a	159	G
32	2a	163	C
32	2a	174	C
32	2a	182	U
32	2a	189(D)	C

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Mol	Chain	Res	Type
32	2a	189(F)	U
32	2a	189(G)	G
32	2a	189(H)	G
32	2a	189(I)	G
32	2a	189(J)	G
32	2a	195	A
32	2a	197	A
32	2a	202	U
32	2a	203	U
32	2a	216	G
32	2a	217	C
32	2a	240	C
32	2a	247	G
32	2a	251	G
32	2a	258	G
32	2a	266	G
32	2a	267	C
32	2a	280	C
32	2a	281	G
32	2a	289	G
32	2a	300	A
32	2a	305	G
32	2a	321	A
32	2a	328	C
32	2a	330	C
32	2a	332	G
32	2a	345	C
32	2a	350	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	375	U
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	417	C

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Mol	Chain	Res	Type
32	2a	421	U
32	2a	422	C
32	2a	423	G
32	2a	424	G
32	2a	429	U
32	2a	430	A
32	2a	438	G
32	2a	439	A
32	2a	442	C
32	2a	451	A
32	2a	452	A
32	2a	470	C
32	2a	471	G
32	2a	484	G
32	2a	485	G
32	2a	491	G
32	2a	496	A
32	2a	498	U
32	2a	505	G
32	2a	506	G
32	2a	510	A
32	2a	511	C
32	2a	518	C
32	2a	524	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	561	U
32	2a	563	A
32	2a	568	G
32	2a	572	A
32	2a	573	A
32	2a	576	G
32	2a	577	G
32	2a	595	G
32	2a	596	C
32	2a	618	C
32	2a	630	G
32	2a	638	G

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Mol	Chain	Res	Type
32	2a	650	G
32	2a	652	U
32	2a	653	A
32	2a	665	A
32	2a	687	A
32	2a	688	G
32	2a	695	A
32	2a	723	U
32	2a	724	G
32	2a	731	G
32	2a	733	A
32	2a	734	G
32	2a	746	A
32	2a	749	C
32	2a	753	A
32	2a	755	G
32	2a	776	G
32	2a	777	A
32	2a	793	U
32	2a	794	A
32	2a	816	A
32	2a	817	C
32	2a	821	G
32	2a	828	A
32	2a	836	G
32	2a	840	C
32	2a	841	U
32	2a	853	G
32	2a	859	A
32	2a	873	A
32	2a	876	G
32	2a	902	G
32	2a	914	A
32	2a	916	G
32	2a	922	G
32	2a	926	G
32	2a	927	G
32	2a	931	C
32	2a	932	C
32	2a	934	C
32	2a	935	A
32	2a	958	A

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Mol	Chain	Res	Type
32	2a	960	U
32	2a	961	U
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	982	U
32	2a	992	U
32	2a	993	G
32	2a	997	U
32	2a	998	G
32	2a	1002	G
32	2a	1005	A
32	2a	1006	C
32	2a	1008	C
32	2a	1009	G
32	2a	1011	G
32	2a	1017	G
32	2a	1020	U
32	2a	1021	G
32	2a	1022	G
32	2a	1025	U
32	2a	1026	G
32	2a	1027	C
32	2a	1028	C
32	2a	1030	C
32	2a	1030(A)	G
32	2a	1030(C)	G
32	2a	1031	G
32	2a	1032	G
32	2a	1036	G
32	2a	1037	C
32	2a	1038	C
32	2a	1039	C
32	2a	1040	U
32	2a	1042	G
32	2a	1044	A
32	2a	1046	A
32	2a	1051	C
32	2a	1065	U

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Mol	Chain	Res	Type
32	2a	1066	C
32	2a	1068	G
32	2a	1077	G
32	2a	1081	G
32	2a	1094	G
32	2a	1095	U
32	2a	1101	A
32	2a	1117	G
32	2a	1122	U
32	2a	1124	G
32	2a	1125	U
32	2a	1127	G
32	2a	1128	C
32	2a	1129	C
32	2a	1135	U
32	2a	1136	U
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G
32	2a	1140	C
32	2a	1141	C
32	2a	1146	A
32	2a	1147	C
32	2a	1152	A
32	2a	1157	A
32	2a	1158	C
32	2a	1159	U
32	2a	1160	G
32	2a	1161	C
32	2a	1168	A
32	2a	1182	G
32	2a	1183	A
32	2a	1184	G
32	2a	1196	U
32	2a	1197	G
32	2a	1202	G
32	2a	1210	C
32	2a	1212	U
32	2a	1213	A
32	2a	1214	C
32	2a	1215	G
32	2a	1227	A

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Mol	Chain	Res	Type
32	2a	1236	A
32	2a	1238	A
32	2a	1240	U
32	2a	1241	G
32	2a	1255	G
32	2a	1256	A
32	2a	1257	U
32	2a	1260	C
32	2a	1267	C
32	2a	1272	G
32	2a	1273	G
32	2a	1275	A
32	2a	1276	G
32	2a	1278	U
32	2a	1279	A
32	2a	1280	A
32	2a	1286	A
32	2a	1287	A
32	2a	1299	A
32	2a	1301	U
32	2a	1302	U
32	2a	1303	C
32	2a	1305	G
32	2a	1312	G
32	2a	1313	U
32	2a	1316	G
32	2a	1320	C
32	2a	1338	G
32	2a	1340	A
32	2a	1346	A
32	2a	1347	G
32	2a	1353	G
32	2a	1363	C
32	2a	1363(A)	A
32	2a	1364	U
32	2a	1370	G
32	2a	1379	G
32	2a	1397	C
32	2a	1398	A
32	2a	1400	5MC
32	2a	1419	G
32	2a	1442	G

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Mol	Chain	Res	Type
32	2a	1442(A)	G
32	2a	1442(B)	A
32	2a	1446	U
32	2a	1447	A
32	2a	1452	C
32	2a	1456	G
32	2a	1457	G
32	2a	1475	G
32	2a	1487	G
32	2a	1492	A
32	2a	1493	A
32	2a	1494	G
32	2a	1503	A
32	2a	1504	G
32	2a	1506	U
32	2a	1507	A
32	2a	1517	G
32	2a	1520	G
32	2a	1529	G
32	2a	1530	G
32	2a	1531	A
32	2a	1532	U
53	2v	13	A
53	2v	14	A
53	2v	15	A
53	2v	19	U
53	2v	24	A
54	2x	9	G
54	2x	20	U
54	2x	21	A
54	2x	22	G
54	2x	31	G
54	2x	47	U
54	2x	48	C
54	2x	52	G
54	2x	56	C
54	2x	67	C
54	2x	68	C

All (48) RNA pucker outliers are listed below:

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Mol	Chain	Res	Type
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Mol	Chain	Res	Type
1	1A	249	C
1	1A	266	G
1	1A	278	A
1	1A	764	A
1	1A	774	A
1	1A	895	U
1	1A	1065	U
1	1A	1067	A
1	1A	1073	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	1653	G
1	1A	1992	G
1	1A	2134	A
1	1A	2170	A
1	1A	2181	G
1	1A	2183	C
1	1A	2406	U
1	1A	2439	A
1	1A	2629	A
1	1A	2689	U
1	1A	2756	U
1	2A	195	A
1	2A	228	A
1	2A	266	G
1	2A	271(K)	U
1	2A	271(M)	G
1	2A	277	C
1	2A	479	A
1	2A	528	A
1	2A	752	A
1	2A	856	C
1	2A	883	G
1	2A	900	A
1	2A	1210	A
1	2A	1420	U
1	2A	1442	G

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Mol	Chain	Res	Type
1	2A	1913	A
1	2A	1992	G
1	2A	2119	A
1	2A	2126	A
1	2A	2286	A
1	2A	2585	U
1	2A	2689	U

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

56 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	2MG	2a	1207	32	19,26,27	1.30	2 (10%)	21,38,41	2.18	7 (33%)
32	MA6	1a	1518	32	19,26,27	1.03	1 (5%)	18,38,41	1.71	6 (33%)
32	5MC	1a	1400	32	15,22,23	1.34	1 (6%)	19,32,35	1.38	3 (15%)
32	2MG	1a	1207	32	19,26,27	1.21	2 (10%)	21,38,41	2.44	9 (42%)
1	5MC	2A	1942	1	15,22,23	1.35	1 (6%)	19,32,35	1.34	3 (15%)
1	PSU	2A	1911	1	17,21,22	1.44	2 (11%)	20,30,33	3.14	6 (30%)
1	5MU	1A	1939	1,56	15,22,23	1.15	2 (13%)	16,32,35	1.98	2 (12%)
32	MA6	2a	1519	32	19,26,27	1.03	1 (5%)	18,38,41	1.68	5 (27%)
32	5MC	2a	1400	32	15,22,23	1.44	1 (6%)	19,32,35	1.49	3 (15%)
32	UR3	1a	1498	32	14,22,23	0.75	0	15,32,35	0.76	1 (6%)
32	PSU	2a	516	32,56	17,21,22	1.59	3 (17%)	20,30,33	3.21	7 (35%)
1	5MU	2A	1915	1,56	15,22,23	1.10	1 (6%)	16,32,35	1.86	2 (12%)
32	5MC	1a	967	32	15,22,23	1.22	1 (6%)	19,32,35	1.33	2 (10%)
32	5MC	2a	1407	32	15,22,23	1.30	1 (6%)	19,32,35	1.30	2 (10%)
1	5MU	1A	1915	1	15,22,23	1.07	1 (6%)	16,32,35	1.75	1 (6%)
32	7MG	1a	527	32,56	22,26,27	1.81	4 (18%)	28,39,42	2.76	9 (32%)
54	PSU	2x	55	54	17,21,22	1.44	2 (11%)	20,30,33	3.26	6 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	7MG	2a	527	32	22,26,27	1.76	4 (18%)	28,39,42	2.69	9 (32%)
54	PSU	1x	55	54,56	17,21,22	1.58	2 (11%)	20,30,33	3.04	6 (30%)
32	5MC	2a	967	32	15,22,23	1.38	1 (6%)	19,32,35	1.36	3 (15%)
1	OMG	1A	2251	1,54,56	18,26,27	1.25	2 (11%)	20,38,41	2.11	6 (30%)
1	PSU	1A	2605	1,56	17,21,22	1.49	3 (17%)	20,30,33	3.19	7 (35%)
32	5MC	1a	1404	32	15,22,23	1.26	1 (6%)	19,32,35	1.44	2 (10%)
54	5MC	1x	32	54	15,22,23	1.37	1 (6%)	19,32,35	1.37	3 (15%)
32	M2G	1a	966	32	20,27,28	1.36	3 (15%)	22,40,43	2.15	6 (27%)
32	5MC	2a	1404	32	15,22,23	1.33	1 (6%)	19,32,35	1.34	3 (15%)
1	PSU	1A	1917	1	17,21,22	1.49	3 (17%)	20,30,33	2.98	5 (25%)
1	5MC	1A	1962	1,56	15,22,23	1.35	1 (6%)	19,32,35	1.26	3 (15%)
32	MA6	1a	1519	32	19,26,27	1.06	1 (5%)	18,38,41	1.64	4 (22%)
1	PSU	2A	1917	1	17,21,22	1.47	2 (11%)	20,30,33	3.04	6 (30%)
43	0TD	1l	92	43	4,9,10	3.15	1 (25%)	3,11,13	2.21	1 (33%)
32	PSU	1a	516	32,56	17,21,22	1.55	3 (17%)	20,30,33	3.10	5 (25%)
32	UR3	2a	1498	32,56	14,22,23	0.76	0	15,32,35	0.72	0
32	4OC	1a	1402	32	16,23,24	0.69	0	17,32,35	1.59	1 (5%)
1	2MU	2A	2552	1,56	14,22,24	0.94	0	14,31,36	0.85	0
1	5MC	2A	1962	1,56	15,22,23	1.29	1 (6%)	19,32,35	1.38	3 (15%)
54	4SU	1x	8	54	14,21,22	1.41	2 (14%)	15,30,33	2.54	2 (13%)
32	5MC	1a	1407	32	15,22,23	1.31	1 (6%)	19,32,35	1.37	2 (10%)
1	PSU	1A	1911	1	17,21,22	1.43	2 (11%)	20,30,33	3.23	5 (25%)
1	5MC	1A	1942	1	15,22,23	1.31	1 (6%)	19,32,35	1.31	3 (15%)
32	4OC	2a	1402	32	16,23,24	0.62	0	17,32,35	1.26	1 (5%)
54	5MU	1x	54	54	15,22,23	1.08	1 (6%)	16,32,35	1.96	2 (12%)
32	M2G	2a	966	32	20,27,28	1.51	3 (15%)	22,40,43	2.13	6 (27%)
1	2MU	1A	2552	1,56	14,22,24	0.86	0	14,31,36	0.99	1 (7%)
54	5MU	2x	54	54	15,22,23	1.09	1 (6%)	16,32,35	1.70	2 (12%)
1	4OC	1A	1920	1	15,22,24	0.76	1 (6%)	17,31,35	1.60	3 (17%)
1	2MA	2A	2503	1,56	17,25,26	1.46	2 (11%)	19,37,40	2.26	3 (15%)
1	2MA	1A	2503	1,56	17,25,26	1.21	2 (11%)	19,37,40	2.12	3 (15%)
1	OMG	2A	2251	1,54,56	18,26,27	1.03	2 (11%)	20,38,41	1.96	5 (25%)
1	PSU	2A	2605	1	17,21,22	1.50	3 (17%)	20,30,33	2.97	6 (30%)
1	5MU	2A	1939	1	15,22,23	1.07	1 (6%)	16,32,35	1.70	2 (12%)
54	4SU	2x	8	54	14,21,22	1.32	2 (14%)	15,30,33	2.03	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	MA6	2a	1518	32	19,26,27	0.99	1 (5%)	18,38,41	1.77	6 (33%)
1	4OC	2A	1920	1	15,22,24	0.75	0	17,31,35	1.26	2 (11%)
54	5MC	2x	32	54	15,22,23	1.20	1 (6%)	19,32,35	1.52	3 (15%)
43	0TD	2l	92	43	4,9,10	3.18	1 (25%)	3,11,13	0.78	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	2MG	2a	1207	32	-	0/5/27/28	0/3/3/3
32	MA6	1a	1518	32	-	2/7/29/30	0/3/3/3
32	5MC	1a	1400	32	-	2/5/25/26	0/2/2/2
32	2MG	1a	1207	32	-	2/5/27/28	0/3/3/3
1	5MC	2A	1942	1	-	0/5/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	1,56	-	0/5/25/26	0/2/2/2
32	MA6	2a	1519	32	-	4/7/29/30	0/3/3/3
32	5MC	2a	1400	32	-	2/5/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/5/25/26	0/2/2/2
32	PSU	2a	516	32,56	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1,56	-	0/5/25/26	0/2/2/2
32	5MC	1a	967	32	-	1/5/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/5/25/26	0/2/2/2
1	5MU	1A	1915	1	-	0/5/25/26	0/2/2/2
32	7MG	1a	527	32,56	-	2/7/37/38	0/3/3/3
54	PSU	2x	55	54	-	0/7/25/26	0/2/2/2
32	7MG	2a	527	32	-	2/7/37/38	0/3/3/3
54	PSU	1x	55	54,56	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	1/5/25/26	0/2/2/2
1	OMG	1A	2251	1,54,56	-	0/5/27/28	0/3/3/3
1	PSU	1A	2605	1,56	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/5/25/26	0/2/2/2
54	5MC	1x	32	54	-	0/5/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/7/29/30	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
1	5MC	1A	1962	1,56	-	2/5/25/26	0/2/2/2
32	MA6	1a	1519	32	-	3/7/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	2A	1917	1	-	1/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	1/3/12/14	-
32	PSU	1a	516	32,56	-	3/7/25/26	0/2/2/2
32	UR3	2a	1498	32,56	-	0/5/25/26	0/2/2/2
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
1	2MU	2A	2552	1,56	-	1/7/27/28	0/2/2/2
1	5MC	2A	1962	1,56	-	2/5/25/26	0/2/2/2
54	4SU	1x	8	54	-	0/5/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/5/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
1	5MC	1A	1942	1	-	0/5/25/26	0/2/2/2
32	4OC	2a	1402	32	-	3/9/29/30	0/2/2/2
54	5MU	1x	54	54	-	0/5/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
1	2MU	1A	2552	1,56	-	0/7/27/28	0/2/2/2
54	5MU	2x	54	54	-	0/5/25/26	0/2/2/2
1	4OC	1A	1920	1	-	1/7/27/30	0/2/2/2
1	2MA	2A	2503	1,56	-	1/3/25/26	0/3/3/3
1	2MA	1A	2503	1,56	-	2/3/25/26	0/3/3/3
1	OMG	2A	2251	1,54,56	-	0/5/27/28	0/3/3/3
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	1	-	2/5/25/26	0/2/2/2
54	4SU	2x	8	54	-	1/5/25/26	0/2/2/2
32	MA6	2a	1518	32	-	1/7/29/30	0/3/3/3
1	4OC	2A	1920	1	-	1/7/27/30	0/2/2/2
54	5MC	2x	32	54	-	0/5/25/26	0/2/2/2
43	0TD	2l	92	43	-	1/3/12/14	-

All (83) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-6.05	1.69	1.84
43	2l	92	0TD	CB-SB	-6.05	1.69	1.84
32	2a	1400	5MC	C5-C4	5.08	1.49	1.41
1	2A	2503	2MA	C6-C5	5.03	1.49	1.41
54	1x	32	5MC	C5-C4	4.91	1.49	1.41
32	2a	967	5MC	C5-C4	4.89	1.48	1.41
32	2a	527	7MG	C6-C5	4.88	1.48	1.41
1	2A	1942	5MC	C5-C4	4.83	1.48	1.41
32	1a	1400	5MC	C5-C4	4.80	1.48	1.41
32	2a	1404	5MC	C5-C4	4.80	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1962	5MC	C5-C4	4.76	1.48	1.41
54	1x	55	PSU	C5-C1'	-4.66	1.48	1.52
32	1a	527	7MG	C6-C5	4.64	1.47	1.41
1	2A	1962	5MC	C5-C4	4.61	1.48	1.41
1	1A	1942	5MC	C5-C4	4.60	1.48	1.41
32	1a	1407	5MC	C5-C4	4.57	1.48	1.41
32	2a	1407	5MC	C5-C4	4.56	1.48	1.41
32	2a	1207	2MG	C6-C5	4.51	1.49	1.41
32	1a	1404	5MC	C5-C4	4.49	1.48	1.41
32	1a	527	7MG	C5-C4	4.46	1.47	1.39
32	1a	967	5MC	C5-C4	4.39	1.48	1.41
32	2a	527	7MG	C5-C4	4.37	1.47	1.39
54	2x	32	5MC	C5-C4	4.33	1.48	1.41
32	2a	516	PSU	C5-C1'	-4.32	1.48	1.52
32	1a	966	M2G	C6-C5	4.22	1.48	1.41
32	2a	966	M2G	C6-C5	4.20	1.48	1.41
32	1a	1207	2MG	C6-C5	4.16	1.48	1.41
1	1A	2251	OMG	C6-C5	4.13	1.48	1.41
1	2A	2605	PSU	C5-C1'	-3.99	1.48	1.52
1	1A	2503	2MA	C6-C5	3.97	1.47	1.41
32	1a	516	PSU	C5-C1'	-3.96	1.48	1.52
54	2x	8	4SU	C4-S4	-3.94	1.60	1.67
32	2a	966	M2G	C2-N2	3.94	1.41	1.34
1	1A	1917	PSU	C5-C1'	-3.85	1.49	1.52
54	2x	55	PSU	C4-C5	3.78	1.49	1.41
32	1a	527	7MG	C5-N7	-3.77	1.33	1.39
54	1x	8	4SU	C4-S4	-3.66	1.60	1.67
1	2A	1917	PSU	C4-C5	3.65	1.49	1.41
1	1A	1911	PSU	C4-C5	3.58	1.49	1.41
54	1x	8	4SU	C2-N3	-3.53	1.31	1.38
1	1A	2605	PSU	C4-C5	3.47	1.48	1.41
32	1a	516	PSU	C4-C5	3.47	1.48	1.41
54	2x	54	5MU	C4-C5	3.47	1.48	1.41
32	2a	516	PSU	C4-C5	3.45	1.48	1.41
1	2A	1915	5MU	C4-C5	3.44	1.48	1.41
1	2A	1911	PSU	C4-C5	3.43	1.48	1.41
1	1A	2605	PSU	C5-C1'	-3.43	1.49	1.52
1	1A	1939	5MU	C4-C5	3.41	1.48	1.41
1	2A	1911	PSU	C5-C1'	-3.40	1.49	1.52
54	1x	54	5MU	C4-C5	3.39	1.48	1.41
1	2A	1917	PSU	C5-C1'	-3.39	1.49	1.52
1	1A	1915	5MU	C4-C5	3.37	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2a	527	7MG	C5-N7	-3.32	1.34	1.39
1	2A	1939	5MU	C4-C5	3.30	1.48	1.41
1	2A	2251	OMG	C6-C5	3.20	1.46	1.41
32	1a	966	M2G	C2-N2	3.17	1.40	1.34
1	2A	2605	PSU	C4-C5	3.13	1.48	1.41
54	1x	55	PSU	C4-C5	3.12	1.48	1.41
54	2x	55	PSU	C5-C1'	-3.12	1.49	1.52
1	1A	1917	PSU	C4-C5	3.10	1.48	1.41
1	1A	1911	PSU	C5-C1'	-3.06	1.49	1.52
1	1A	2251	OMG	C5-C4	2.64	1.47	1.40
32	2a	1519	MA6	C5-C4	2.61	1.47	1.40
32	2a	966	M2G	C5-C4	2.57	1.47	1.40
32	2a	1207	2MG	C5-C4	2.56	1.47	1.40
32	1a	1519	MA6	C5-C4	2.54	1.47	1.40
32	1a	527	7MG	C4-N9	-2.54	1.33	1.38
32	1a	1518	MA6	C5-C4	2.51	1.47	1.40
32	2a	1518	MA6	C5-C4	2.50	1.47	1.40
1	2A	2251	OMG	C5-C4	2.47	1.47	1.40
32	2a	527	7MG	C4-N9	-2.46	1.33	1.38
32	2a	516	PSU	O4'-C1'	-2.46	1.40	1.44
1	2A	2503	2MA	C5-C4	2.42	1.47	1.40
32	1a	966	M2G	C5-C4	2.32	1.47	1.40
32	1a	1207	2MG	C5-C4	2.32	1.47	1.40
54	2x	8	4SU	C2-N3	-2.23	1.33	1.38
1	1A	1939	5MU	C2-N3	-2.22	1.33	1.38
1	1A	2605	PSU	C2-N3	-2.21	1.33	1.38
1	1A	2503	2MA	C5-C4	2.12	1.46	1.40
1	2A	2605	PSU	C2-N3	-2.11	1.34	1.38
32	1a	516	PSU	O4'-C1'	-2.08	1.41	1.44
1	1A	1917	PSU	O4'-C1'	-2.08	1.41	1.44
1	1A	1920	4OC	C6-N1	-2.04	1.33	1.35

All (206) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2x	55	PSU	N1-C2-N3	-9.26	121.07	128.43
1	1A	1911	PSU	N1-C2-N3	-9.18	121.13	128.43
1	1A	2605	PSU	N1-C2-N3	-9.09	121.20	128.43
32	1a	527	7MG	N3-C4-N9	9.08	138.57	126.91
32	2a	516	PSU	N1-C2-N3	-8.92	121.34	128.43
1	2A	1911	PSU	N1-C2-N3	-8.77	121.45	128.43
32	1a	516	PSU	N1-C2-N3	-8.49	121.68	128.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	527	7MG	N3-C4-N9	8.46	137.77	126.91
54	1x	8	4SU	C2-N3-C4	8.45	127.40	115.15
1	1A	1917	PSU	N1-C2-N3	-8.14	121.96	128.43
1	2A	2605	PSU	N1-C2-N3	-8.05	122.03	128.43
54	1x	55	PSU	N1-C2-N3	-7.88	122.16	128.43
1	2A	1917	PSU	N1-C2-N3	-7.86	122.18	128.43
1	2A	2503	2MA	C2-N3-C4	7.69	121.77	115.52
54	1x	54	5MU	C4-N3-C2	7.29	121.29	115.14
1	1A	1911	PSU	C4-N3-C2	7.15	121.18	115.14
54	2x	55	PSU	C4-N3-C2	7.08	121.12	115.14
1	2A	1911	PSU	C4-N3-C2	7.00	121.05	115.14
1	1A	1939	5MU	C4-N3-C2	6.90	120.97	115.14
1	1A	2503	2MA	C2-N3-C4	6.89	121.12	115.52
32	1a	516	PSU	C4-N3-C2	6.73	120.83	115.14
32	2a	516	PSU	C4-N3-C2	6.71	120.81	115.14
1	1A	1917	PSU	C4-N3-C2	6.69	120.79	115.14
1	2A	1915	5MU	C4-N3-C2	6.66	120.77	115.14
1	2A	1917	PSU	C4-N3-C2	6.55	120.67	115.14
1	1A	1915	5MU	C4-N3-C2	6.53	120.65	115.14
1	1A	2605	PSU	C4-N3-C2	6.46	120.60	115.14
54	2x	8	4SU	C2-N3-C4	6.41	124.44	115.15
54	2x	54	5MU	C4-N3-C2	6.17	120.35	115.14
54	1x	55	PSU	C4-N3-C2	6.08	120.28	115.14
1	2A	2605	PSU	C4-N3-C2	6.07	120.27	115.14
1	2A	1939	5MU	C4-N3-C2	5.60	119.87	115.14
32	1a	1402	4OC	CM4-N4-C4	-5.47	118.27	122.97
32	2a	527	7MG	N7-C8-N9	-5.43	95.61	103.38
1	1A	2251	OMG	C2-N3-C4	5.42	121.55	115.36
32	2a	966	M2G	C6-N1-C2	5.35	122.55	116.18
32	1a	516	PSU	C5-C4-N3	-5.34	118.48	125.36
1	2A	1917	PSU	C5-C4-N3	-5.33	118.49	125.36
1	1A	1917	PSU	C5-C4-N3	-5.32	118.51	125.36
1	1A	1911	PSU	C5-C4-N3	-5.25	118.59	125.36
54	1x	55	PSU	C5-C4-N3	-5.25	118.60	125.36
32	2a	516	PSU	C5-C4-N3	-5.24	118.61	125.36
1	2A	1911	PSU	C5-C4-N3	-5.22	118.64	125.36
32	2a	966	M2G	C2-N3-C4	5.21	121.20	115.28
32	1a	527	7MG	C5-C4-N3	-5.12	118.14	126.49
32	1a	966	M2G	C6-N1-C2	5.11	122.26	116.18
32	1a	527	7MG	N7-C8-N9	-5.06	96.15	103.38
54	2x	55	PSU	C5-C4-N3	-5.00	118.92	125.36
32	1a	1207	2MG	C6-C5-C4	-4.94	116.08	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	527	7MG	C5-C4-N3	-4.76	118.72	126.49
1	2A	2605	PSU	C5-C4-N3	-4.72	119.28	125.36
32	2a	527	7MG	C6-N1-C2	4.71	123.42	115.93
32	1a	966	M2G	C2-N3-C4	4.71	120.62	115.28
54	1x	55	PSU	C5-C6-N1	-4.71	118.66	124.44
1	1A	1920	4OC	C2-N3-C4	4.70	121.10	116.34
32	2a	1207	2MG	C2-N3-C4	4.65	120.56	115.28
32	1a	1207	2MG	C6-N1-C2	4.61	123.43	115.18
54	1x	8	4SU	C5-C4-N3	-4.61	117.67	123.83
32	1a	527	7MG	C6-C5-C4	4.55	120.08	115.20
1	1A	2605	PSU	C6-N1-C2	4.50	122.79	115.36
1	2A	2605	PSU	C5-C6-N1	-4.48	118.94	124.44
1	1A	2605	PSU	C5-C4-N3	-4.45	119.63	125.36
54	2x	55	PSU	C6-N1-C2	4.42	122.65	115.36
32	1a	527	7MG	C6-N1-C2	4.37	122.88	115.93
32	2a	516	PSU	C5-C6-N1	-4.34	119.10	124.44
1	1A	1911	PSU	C6-N1-C2	4.34	122.52	115.36
1	2A	2503	2MA	C5-C6-N1	-4.34	118.51	123.06
32	1a	1207	2MG	C2-N3-C4	4.31	120.17	115.28
1	2A	2251	OMG	C2-N3-C4	4.30	120.27	115.36
32	2a	516	PSU	C6-N1-C2	4.29	122.44	115.36
1	1A	2503	2MA	C5-C6-N1	-4.28	118.58	123.06
32	2a	1207	2MG	C5-C6-N1	-4.24	117.63	123.43
32	2a	966	M2G	C5-C6-N1	-4.24	117.64	123.43
32	1a	1207	2MG	C5-C6-N1	-4.22	117.66	123.43
1	1A	2605	PSU	C5-C6-N1	-4.17	119.32	124.44
54	2x	55	PSU	C5-C6-N1	-4.16	119.33	124.44
1	2A	1917	PSU	C5-C6-N1	-4.14	119.35	124.44
32	1a	516	PSU	C6-N1-C2	4.14	122.18	115.36
32	1a	966	M2G	C5-C6-N1	-4.13	117.78	123.43
32	1a	1407	5MC	C2-N3-C4	4.12	121.00	116.02
1	2A	2605	PSU	C6-N1-C2	4.12	122.16	115.36
32	1a	1404	5MC	C2-N3-C4	4.09	120.95	116.02
1	2A	1911	PSU	C6-N1-C2	4.08	122.09	115.36
54	2x	32	5MC	C2-N3-C4	4.06	120.91	116.02
54	1x	55	PSU	C6-N1-C2	4.03	122.01	115.36
32	1a	516	PSU	C5-C6-N1	-4.03	119.48	124.44
1	2A	1920	4OC	C2-N3-C4	4.01	120.40	116.34
1	2A	1917	PSU	C6-N1-C2	3.98	121.92	115.36
32	2a	1207	2MG	C6-N1-C2	3.98	122.30	115.18
32	2a	527	7MG	C6-C5-C4	3.97	119.47	115.20
1	1A	1911	PSU	C5-C6-N1	-3.93	119.61	124.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2251	OMG	C6-N1-C2	3.88	122.09	115.93
32	2a	1404	5MC	C2-N3-C4	3.88	120.70	116.02
32	2a	1207	2MG	C6-C5-C4	-3.86	117.11	120.80
32	2a	527	7MG	C5-C6-N1	-3.85	115.22	123.14
1	1A	2251	OMG	C5-C6-N1	-3.85	118.17	123.43
1	2A	2251	OMG	C5-C6-N1	-3.85	118.17	123.43
1	2A	1911	PSU	C5-C6-N1	-3.82	119.74	124.44
32	1a	967	5MC	C2-N3-C4	3.78	120.58	116.02
1	1A	2251	OMG	C6-N1-C2	3.77	121.91	115.93
32	2a	967	5MC	C2-N3-C4	3.76	120.56	116.02
32	1a	527	7MG	C5-C6-N1	-3.75	115.44	123.14
1	1A	1917	PSU	C6-N1-C2	3.74	121.54	115.36
54	2x	8	4SU	C5-C4-N3	-3.73	118.83	123.83
32	2a	1519	MA6	N1-C6-N6	3.71	120.96	117.06
32	1a	966	M2G	C6-C5-C4	-3.70	117.26	120.80
32	2a	1402	4OC	CM4-N4-C4	-3.69	119.80	122.97
32	2a	1407	5MC	C2-N3-C4	3.69	120.47	116.02
1	1A	1917	PSU	C5-C6-N1	-3.67	119.93	124.44
32	2a	1400	5MC	C2-N3-C4	3.60	120.37	116.02
1	2A	1962	5MC	C2-N3-C4	3.54	120.29	116.02
43	1l	92	0TD	CSB-SB-CB	3.52	108.77	101.85
32	2a	1518	MA6	C9-N6-C6	-3.50	108.92	119.51
54	1x	32	5MC	C2-N3-C4	3.50	120.24	116.02
32	1a	1518	MA6	C4-C5-N7	-3.44	105.81	109.40
32	1a	1518	MA6	N3-C2-N1	-3.40	123.36	128.68
32	1a	1400	5MC	C2-N3-C4	3.35	120.06	116.02
32	1a	1519	MA6	C4-C5-N7	-3.34	105.92	109.40
1	2A	2503	2MA	C4-C5-N7	-3.32	105.94	109.40
32	1a	1518	MA6	C9-N6-C6	-3.31	109.50	119.51
1	1A	1962	5MC	C2-N3-C4	3.27	119.97	116.02
54	1x	55	PSU	C5-C1'-C2'	-3.26	109.51	115.32
1	2A	1942	5MC	C2-N3-C4	3.25	119.94	116.02
1	2A	2251	OMG	C6-C5-C4	-3.24	117.70	120.80
54	2x	32	5MC	N4-C4-N3	3.21	121.57	117.03
32	1a	1404	5MC	N4-C4-N3	3.20	121.56	117.03
32	2a	1518	MA6	N3-C2-N1	-3.18	123.71	128.68
32	1a	1207	2MG	CM2-N2-C2	-3.17	119.76	123.59
1	2A	1917	PSU	C5-C1'-C2'	-3.17	109.66	115.32
32	1a	1519	MA6	N3-C2-N1	-3.16	123.74	128.68
1	1A	1942	5MC	C2-N3-C4	3.15	119.83	116.02
1	1A	2251	OMG	N3-C2-N1	-3.14	123.03	127.22
32	2a	1519	MA6	N3-C2-N1	-3.05	123.92	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1518	MA6	N1-C6-N6	3.03	120.24	117.06
1	2A	2251	OMG	N3-C2-N1	-3.02	123.20	127.22
32	2a	1518	MA6	C4-C5-N7	-3.01	106.27	109.40
32	1a	1519	MA6	C9-N6-C6	-3.01	110.41	119.51
32	2a	1519	MA6	C4-C5-N7	-3.00	106.27	109.40
32	2a	966	M2G	C6-C5-C4	-2.98	117.95	120.80
1	2A	1939	5MU	C5-C6-N1	-2.96	119.01	122.19
1	1A	1939	5MU	C5-C6-N1	-2.96	119.01	122.19
32	1a	1519	MA6	N1-C6-N6	2.94	120.15	117.06
32	2a	1207	2MG	C4-C5-N7	-2.92	106.36	109.40
1	2A	1942	5MC	C5-C6-N1	-2.91	119.06	122.19
1	1A	1920	4OC	N4-C4-N3	2.90	121.07	116.49
1	1A	2251	OMG	C6-C5-C4	-2.89	118.03	120.80
32	1a	1207	2MG	C4-C5-N7	-2.88	106.40	109.40
32	1a	966	M2G	C4-C5-N7	-2.88	106.40	109.40
1	1A	1942	5MC	C5-C6-N1	-2.88	119.09	122.19
32	2a	1207	2MG	CM2-N2-C2	-2.87	120.13	123.59
32	1a	1207	2MG	C1'-N9-C4	-2.86	121.62	126.64
1	2A	1962	5MC	N4-C4-N3	2.82	121.02	117.03
32	2a	1519	MA6	C9-N6-C6	-2.82	110.98	119.51
32	2a	527	7MG	C8-N7-C5	2.81	116.25	108.94
1	1A	1962	5MC	C5-C6-N1	-2.76	119.22	122.19
1	1A	2503	2MA	C4-C5-N7	-2.75	106.53	109.40
1	1A	2605	PSU	C5-C1'-C2'	-2.74	110.44	115.32
32	2a	1407	5MC	N4-C4-N3	2.73	120.89	117.03
32	1a	1400	5MC	C5-C6-N1	-2.71	119.27	122.19
32	1a	1407	5MC	N4-C4-N3	2.70	120.84	117.03
32	2a	1400	5MC	C5-C6-N1	-2.65	119.33	122.19
32	1a	527	7MG	C8-N7-C5	2.64	115.81	108.94
54	1x	32	5MC	C5-C6-N1	-2.57	119.42	122.19
32	2a	516	PSU	O4'-C1'-C2'	2.54	108.78	104.66
32	1a	967	5MC	N4-C4-N3	2.47	120.53	117.03
1	2A	1915	5MU	C5-C6-N1	-2.45	119.55	122.19
32	1a	966	M2G	CM2-N2-C2	-2.44	118.96	121.29
32	1a	1207	2MG	N3-C2-N1	-2.44	122.37	126.23
1	2A	2605	PSU	C5-C1'-C2'	-2.43	110.97	115.32
32	2a	1404	5MC	N4-C4-N3	2.43	120.47	117.03
54	2x	32	5MC	CM5-C5-C4	-2.43	119.26	121.72
32	2a	1518	MA6	C10-N6-C6	-2.42	112.18	119.51
1	1A	1962	5MC	N4-C4-N3	2.40	120.42	117.03
1	1A	1942	5MC	N4-C4-N3	2.38	120.39	117.03
32	1a	1207	2MG	N2-C2-N1	2.37	119.24	116.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1920	4OC	C5-C4-N3	-2.35	119.01	121.72
32	2a	967	5MC	N4-C4-N3	2.32	120.32	117.03
1	2A	1942	5MC	N4-C4-N3	2.32	120.31	117.03
32	2a	966	M2G	C4-C5-N7	-2.31	106.99	109.40
32	2a	1518	MA6	C10-N6-C9	-2.30	108.72	116.12
32	1a	1400	5MC	N4-C4-N3	2.26	120.23	117.03
1	1A	2251	OMG	C4-C5-N7	-2.26	107.05	109.40
32	2a	1519	MA6	C10-N6-C6	-2.25	112.69	119.51
32	1a	527	7MG	C5-C4-N9	-2.25	103.28	106.44
32	2a	967	5MC	C5-C6-N1	-2.25	119.77	122.19
32	2a	966	M2G	N3-C2-N2	2.23	119.44	117.18
1	2A	1911	PSU	C5-C1'-C2'	-2.23	111.34	115.32
32	1a	1518	MA6	C10-N6-C9	-2.22	108.96	116.12
1	2A	1920	4OC	N4-C4-N3	2.20	119.97	116.49
32	2a	1400	5MC	N4-C4-N3	2.20	120.14	117.03
32	2a	1404	5MC	C5-C6-N1	-2.18	119.84	122.19
54	1x	32	5MC	N4-C4-N3	2.16	120.08	117.03
54	2x	54	5MU	C5-C6-N1	-2.15	119.88	122.19
54	1x	54	5MU	C5-C6-N1	-2.14	119.89	122.19
32	2a	1207	2MG	N2-C2-N1	2.14	119.01	116.96
32	1a	1518	MA6	N1-C6-N6	2.14	119.31	117.06
32	2a	527	7MG	CM7-N7-C5	2.11	132.13	124.01
1	1A	2552	2MU	C5-C4-N3	-2.11	118.66	123.31
32	2a	527	7MG	C5-C4-N9	-2.11	103.49	106.44
32	2a	516	PSU	C5-C1'-C2'	-2.10	111.57	115.32
1	1A	2605	PSU	O2'-C2'-C1'	-2.06	107.04	111.94
32	1a	1518	MA6	C10-N6-C6	-2.05	113.31	119.51
32	1a	1498	UR3	C3U-N3-C4	2.05	120.83	118.12
54	2x	55	PSU	C5-C1'-C2'	-2.04	111.69	115.32
32	1a	527	7MG	C2-N3-C4	2.04	119.52	113.89
1	2A	1962	5MC	C5-C6-N1	-2.03	120.01	122.19

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	1518	MA6	C5-C6-N6-C10
32	1a	1400	5MC	O4'-C4'-C5'-O5'
32	1a	1400	5MC	C3'-C4'-C5'-O5'
32	1a	1207	2MG	N1-C2-N2-CM2
32	1a	1207	2MG	N3-C2-N2-CM2
32	2a	1519	MA6	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
32	2a	527	7MG	C3'-C4'-C5'-O5'
1	2A	1962	5MC	O4'-C1'-N1-C6
1	2A	1962	5MC	C2'-C1'-N1-C6
1	1A	1962	5MC	O4'-C1'-N1-C6
1	1A	1962	5MC	C2'-C1'-N1-C6
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	1a	1519	MA6	C5-C6-N6-C10
43	1l	92	0TD	CG-CB-SB-CSB
32	2a	1402	4OC	O4'-C4'-C5'-O5'
32	2a	1402	4OC	C2'-C1'-N1-C6
1	1A	1920	4OC	C2'-C1'-N1-C6
1	2A	1939	5MU	C2'-C1'-N1-C6
1	2A	1939	5MU	O4'-C1'-N1-C6
54	2x	8	4SU	C2'-C1'-N1-C6
1	2A	1920	4OC	O4'-C1'-N1-C6
43	2l	92	0TD	CG-CB-SB-CSB
32	2a	1519	MA6	C3'-C4'-C5'-O5'
32	2a	1400	5MC	O4'-C4'-C5'-O5'
32	2a	1400	5MC	C3'-C4'-C5'-O5'
32	1a	527	7MG	C3'-C4'-C5'-O5'
32	2a	1402	4OC	C3'-C4'-C5'-O5'
32	2a	527	7MG	O4'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
32	1a	516	PSU	O4'-C4'-C5'-O5'
32	1a	527	7MG	O4'-C4'-C5'-O5'
32	1a	1518	MA6	C5-C6-N6-C9
32	1a	516	PSU	C3'-C4'-C5'-O5'
32	2a	1519	MA6	C5-C6-N6-C10
32	2a	1518	MA6	C5-C6-N6-C10
32	1a	967	5MC	O4'-C4'-C5'-O5'
1	2A	1917	PSU	O4'-C4'-C5'-O5'
1	1A	2503	2MA	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C4'-C5'-O5'-P
1	1A	2503	2MA	C4'-C5'-O5'-P
32	1a	516	PSU	C2'-C1'-C5-C6
1	2A	2552	2MU	C3'-C2'-O2'-C6'
32	2a	967	5MC	O4'-C4'-C5'-O5'
32	1a	1402	4OC	O4'-C4'-C5'-O5'
1	2A	2503	2MA	O4'-C4'-C5'-O5'
32	1a	1402	4OC	C5-C4-N4-CM4

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 2024 ligands modelled in this entry, 2022 are monoatomic - leaving 2 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	$\# Z > 2$
58	SF4	1d	302	35	0,12,12	0.00	-	-		
58	SF4	2d	302	35	0,12,12	0.00	-	-		

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
58	SF4	1d	302	35	-	-	0/6/5/5
58	SF4	2d	302	35	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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%)	0.17	8 (0%) 94 85	26, 42, 92, 108	0
1	2A	2789/2915 (95%)	0.10	12 (0%) 92 82	35, 59, 90, 106	0
2	1B	120/121 (99%)	-0.16	0 100 100	36, 51, 67, 83	0
2	2B	120/121 (99%)	-0.04	0 100 100	64, 81, 90, 98	0
3	1D	275/276 (99%)	0.48	8 (2%) 51 26	29, 41, 54, 77	0
3	2D	275/276 (99%)	0.59	9 (3%) 46 23	35, 50, 62, 71	0
4	1E	204/206 (99%)	0.11	1 (0%) 91 79	26, 45, 60, 73	0
4	2E	204/206 (99%)	0.21	0 100 100	37, 57, 67, 77	0
5	1F	203/210 (96%)	-0.04	0 100 100	28, 47, 65, 79	0
5	2F	203/210 (96%)	0.15	5 (2%) 57 32	37, 65, 77, 81	0
6	1G	181/182 (99%)	-0.12	0 100 100	42, 58, 70, 83	0
6	2G	181/182 (99%)	0.81	32 (17%) 1 0	69, 79, 86, 92	0
7	1H	174/180 (96%)	-0.25	0 100 100	45, 55, 66, 74	0
7	2H	174/180 (96%)	0.58	20 (11%) 4 1	64, 79, 87, 97	0
8	1I	146/148 (98%)	-0.02	0 100 100	45, 69, 78, 82	0
8	2I	146/148 (98%)	-0.00	3 (2%) 63 39	57, 72, 81, 87	0
9	1N	140/140 (100%)	0.13	1 (0%) 87 72	34, 45, 62, 72	0
9	2N	140/140 (100%)	0.60	8 (5%) 23 10	46, 63, 76, 84	0
10	1O	122/122 (100%)	0.28	0 100 100	34, 44, 58, 64	0
10	2O	122/122 (100%)	0.29	1 (0%) 86 70	45, 56, 69, 74	0
11	1P	149/150 (99%)	0.12	0 100 100	28, 49, 67, 86	0
11	2P	149/150 (99%)	0.63	11 (7%) 14 5	43, 66, 81, 84	0
12	1Q	141/141 (100%)	0.03	1 (0%) 87 72	32, 46, 58, 67	0
12	2Q	141/141 (100%)	0.40	3 (2%) 63 39	47, 63, 75, 80	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	0.01	0 100 100	34, 41, 55, 63	0
13	2R	118/118 (100%)	0.17	0 100 100	40, 53, 61, 67	0
14	1S	110/112 (98%)	-0.07	0 100 100	42, 51, 60, 66	0
14	2S	110/112 (98%)	0.54	7 (6%) 19 7	63, 73, 82, 85	0
15	1T	131/146 (89%)	-0.02	0 100 100	34, 48, 68, 83	0
15	2T	131/146 (89%)	0.09	1 (0%) 86 70	48, 58, 75, 85	0
16	1U	116/118 (98%)	0.27	1 (0%) 84 66	31, 41, 53, 66	0
16	2U	116/118 (98%)	0.52	1 (0%) 84 66	43, 60, 74, 81	0
17	1V	101/101 (100%)	-0.01	0 100 100	32, 47, 60, 73	0
17	2V	101/101 (100%)	0.43	8 (7%) 12 4	43, 68, 77, 81	0
18	1W	112/113 (99%)	0.23	1 (0%) 84 66	32, 40, 55, 76	0
18	2W	112/113 (99%)	0.46	7 (6%) 20 8	42, 52, 64, 87	0
19	1X	95/96 (98%)	0.05	1 (1%) 80 60	32, 41, 58, 70	0
19	2X	95/96 (98%)	0.42	3 (3%) 47 24	53, 63, 74, 84	0
20	1Y	107/110 (97%)	-0.13	1 (0%) 84 66	38, 52, 68, 73	0
20	2Y	107/110 (97%)	0.42	9 (8%) 11 4	58, 69, 78, 83	0
21	1Z	154/206 (74%)	-0.34	0 100 100	46, 62, 77, 80	0
21	2Z	160/206 (77%)	0.02	1 (0%) 89 76	66, 77, 85, 90	0
22	10	76/85 (89%)	-0.01	0 100 100	33, 43, 55, 63	0
22	20	76/85 (89%)	1.19	18 (23%) 0 0	46, 63, 71, 80	0
23	11	97/98 (98%)	0.34	0 100 100	33, 46, 65, 71	0
23	21	97/98 (98%)	0.73	5 (5%) 27 11	43, 55, 72, 76	0
24	12	70/72 (97%)	-0.03	0 100 100	38, 50, 60, 72	0
24	22	70/72 (97%)	-0.05	1 (1%) 75 53	61, 70, 75, 79	0
25	13	59/60 (98%)	0.02	0 100 100	31, 43, 61, 80	0
25	23	59/60 (98%)	0.79	3 (5%) 28 12	51, 65, 74, 82	0
26	14	69/71 (97%)	-0.43	1 (1%) 75 53	55, 69, 83, 89	0
26	24	69/71 (97%)	0.17	6 (8%) 10 3	76, 85, 91, 95	0
27	15	59/60 (98%)	0.22	1 (1%) 70 46	28, 40, 54, 66	0
27	25	59/60 (98%)	0.17	1 (1%) 70 46	40, 52, 63, 72	0
28	16	53/54 (98%)	-0.09	0 100 100	36, 42, 54, 59	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.10	2 (3%) 40 20	52, 60, 66, 77	0
29	17	48/49 (97%)	0.54	2 (4%) 36 17	29, 36, 58, 63	0
29	27	48/49 (97%)	0.81	3 (6%) 20 8	37, 45, 66, 74	0
30	18	64/65 (98%)	0.55	2 (3%) 49 25	29, 39, 48, 57	0
30	28	64/65 (98%)	1.14	10 (15%) 2 1	49, 55, 63, 68	0
31	19	37/37 (100%)	0.38	0 100 100	39, 46, 60, 66	0
31	29	37/37 (100%)	0.61	2 (5%) 25 11	60, 67, 74, 75	0
32	1a	1488/1521 (97%)	-0.04	2 (0%) 95 91	39, 65, 89, 105	0
32	2a	1491/1521 (98%)	0.06	14 (0%) 84 66	49, 75, 93, 105	0
33	1b	231/256 (90%)	-0.12	1 (0%) 92 82	62, 75, 84, 94	0
33	2b	231/256 (90%)	0.61	25 (10%) 5 2	68, 81, 88, 95	0
34	1c	206/239 (86%)	0.15	6 (2%) 51 26	52, 67, 76, 83	0
34	2c	206/239 (86%)	0.65	22 (10%) 6 2	69, 81, 86, 92	0
35	1d	208/209 (99%)	0.27	4 (1%) 66 43	54, 67, 76, 80	0
35	2d	208/209 (99%)	0.70	15 (7%) 15 5	59, 72, 81, 86	0
36	1e	148/162 (91%)	0.66	9 (6%) 21 8	51, 63, 72, 77	0
36	2e	148/162 (91%)	1.11	24 (16%) 1 0	62, 73, 80, 85	0
37	1f	100/101 (99%)	-0.14	0 100 100	53, 63, 73, 74	0
37	2f	100/101 (99%)	-0.15	0 100 100	58, 70, 77, 81	0
38	1g	155/156 (99%)	-0.16	7 (4%) 33 15	56, 66, 78, 86	0
38	2g	155/156 (99%)	0.48	15 (9%) 7 2	67, 77, 83, 88	0
39	1h	137/138 (99%)	0.33	3 (2%) 62 38	57, 66, 73, 79	0
39	2h	137/138 (99%)	0.81	20 (14%) 2 1	61, 72, 79, 80	0
40	1i	127/128 (99%)	0.07	4 (3%) 49 25	51, 71, 80, 85	0
40	2i	127/128 (99%)	1.13	29 (22%) 0 0	72, 82, 87, 91	0
41	1j	97/105 (92%)	-0.04	2 (2%) 63 39	59, 72, 82, 85	0
41	2j	96/105 (91%)	1.12	26 (27%) 0 0	71, 83, 89, 92	0
42	1k	114/129 (88%)	0.45	3 (2%) 56 30	48, 65, 75, 81	0
42	2k	114/129 (88%)	0.60	5 (4%) 34 16	61, 70, 77, 86	0
43	1l	121/132 (91%)	0.30	3 (2%) 57 32	43, 57, 67, 75	0
43	2l	121/132 (91%)	0.48	7 (5%) 23 9	55, 65, 73, 79	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	123/126 (97%)	0.15	5 (4%) 37 18	55, 66, 77, 95	0
44	2m	122/126 (96%)	0.52	11 (9%) 9 3	71, 81, 86, 93	0
45	1n	60/61 (98%)	0.37	3 (5%) 28 12	52, 63, 69, 72	0
45	2n	60/61 (98%)	1.30	18 (30%) 0 0	72, 81, 86, 88	0
46	1o	88/89 (98%)	0.22	0 100 100	48, 63, 75, 81	0
46	2o	88/89 (98%)	0.08	1 (1%) 80 60	61, 71, 78, 85	0
47	1p	82/88 (93%)	0.44	3 (3%) 41 20	58, 66, 76, 86	0
47	2p	82/88 (93%)	0.25	1 (1%) 79 58	54, 68, 76, 82	0
48	1q	99/105 (94%)	0.17	2 (2%) 65 41	53, 65, 74, 77	0
48	2q	99/105 (94%)	0.45	4 (4%) 38 18	60, 68, 75, 80	0
49	1r	68/88 (77%)	0.20	0 100 100	57, 65, 74, 80	0
49	2r	68/88 (77%)	0.44	2 (2%) 51 26	61, 69, 78, 81	0
50	1s	83/93 (89%)	-0.20	0 100 100	57, 66, 77, 82	0
50	2s	83/93 (89%)	0.23	2 (2%) 59 34	75, 82, 89, 93	0
51	1t	96/106 (90%)	0.26	7 (7%) 15 5	58, 68, 79, 83	0
51	2t	96/106 (90%)	0.26	3 (3%) 49 25	56, 68, 79, 82	0
52	1u	23/27 (85%)	0.26	2 (8%) 10 3	59, 64, 69, 71	0
52	2u	23/27 (85%)	1.94	10 (43%) 0 0	72, 78, 83, 88	0
53	1v	13/24 (54%)	2.18	5 (38%) 0 0	52, 88, 95, 95	0
53	2v	13/24 (54%)	2.64	7 (53%) 0 0	65, 95, 100, 102	0
54	1x	72/77 (93%)	0.03	0 100 100	37, 63, 80, 94	0
54	2x	72/77 (93%)	-0.10	0 100 100	51, 77, 89, 94	0
55	1z	16/16 (100%)	1.22	4 (25%) 0 0	37, 43, 62, 75	0
55	2z	16/16 (100%)	1.90	5 (31%) 0 0	48, 52, 72, 77	0
All	All	20628/21476 (96%)	0.21	562 (2%) 54 28	26, 62, 86, 108	0

All (562) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
53	1v	24	A	8.4
44	2m	123	ALA	8.3
38	2g	80	VAL	8.2
44	1m	124	PRO	7.8
44	2m	124	PRO	7.7

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Mol	Chain	Res	Type	RSRZ
32	2a	1532	U	7.0
29	27	48	LYS	6.9
44	1m	123	ALA	6.7
53	2v	24	A	6.3
41	2j	59	SER	6.2
53	1v	23	A	5.9
6	2G	39	ILE	5.5
38	2g	78	ARG	5.4
34	2c	163	ALA	5.4
53	2v	23	A	5.4
38	2g	82	GLY	5.1
55	2z	15	TRP	5.0
55	2z	16	ARG	5.0
7	2H	115	VAL	5.0
6	2G	160	VAL	4.9
7	2H	123	PHE	4.8
36	2e	31	LEU	4.8
6	2G	29	TRP	4.7
53	2v	22	U	4.7
45	2n	37	PHE	4.7
33	2b	232	PRO	4.6
41	2j	48	THR	4.6
55	1z	16	ARG	4.6
39	2h	81	HIS	4.6
41	2j	6	ILE	4.5
52	2u	6	ARG	4.5
44	2m	102	ARG	4.5
41	2j	58	ASP	4.5
45	2n	35	ARG	4.5
38	2g	81	GLY	4.5
6	2G	161	THR	4.4
36	2e	10	MET	4.4
36	2e	13	ILE	4.4
9	2N	10	GLU	4.4
55	2z	13	PRO	4.3
39	2h	80	ILE	4.3
40	2i	123	PRO	4.3
44	2m	120	LYS	4.3
44	1m	122	LYS	4.2
41	2j	67	THR	4.2
36	2e	88	LYS	4.2
34	2c	124	ILE	4.2

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Mol	Chain	Res	Type	RSRZ
1	2A	2145	C	4.2
22	20	69	PHE	4.2
34	2c	13	GLY	4.2
14	2S	58	LEU	4.1
38	2g	79	ARG	4.1
7	2H	128	PRO	4.1
40	2i	124	GLN	4.1
52	2u	13	ILE	4.1
40	2i	64	THR	4.0
39	2h	82	HIS	4.0
3	1D	275	LYS	4.0
6	2G	152	LEU	4.0
36	2e	12	LEU	4.0
53	2v	12	A	3.9
36	2e	8	GLU	3.9
40	2i	26	VAL	3.9
34	2c	152	ILE	3.9
34	2c	201	TYR	3.9
32	2a	1531	A	3.9
16	1U	117	GLN	3.9
42	2k	13	GLN	3.9
17	2V	80	GLN	3.8
42	2k	126	ARG	3.8
34	2c	149	ALA	3.8
6	2G	137	GLU	3.8
23	2l	2	SER	3.8
44	1m	121	LYS	3.8
36	1e	18	ARG	3.8
26	24	54	GLY	3.7
41	2j	61	GLU	3.7
9	2N	8	GLN	3.7
22	20	57	PHE	3.7
3	1D	276	LYS	3.7
36	1e	81	GLU	3.7
20	2Y	1	MET	3.7
43	2l	64	TYR	3.7
44	1m	120	LYS	3.7
41	2j	46	ARG	3.6
38	1g	82	GLY	3.6
29	17	48	LYS	3.5
45	2n	25	VAL	3.5
34	2c	148	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
34	2c	191	THR	3.5
7	2H	107	VAL	3.5
51	1t	20	LEU	3.5
38	1g	84	ASN	3.5
11	2P	45	LEU	3.5
33	2b	188	ALA	3.5
34	2c	14	ILE	3.5
41	2j	50	ILE	3.5
22	20	53	MET	3.5
41	2j	62	HIS	3.5
17	2V	74	LYS	3.5
6	2G	138	GLN	3.5
36	2e	113	ALA	3.5
4	1E	6	GLY	3.5
33	2b	70	PHE	3.4
33	2b	165	VAL	3.4
52	2u	5	ASP	3.4
39	2h	84	ARG	3.4
1	2A	2131	G	3.4
36	1e	88	LYS	3.4
35	2d	164	ALA	3.4
53	2v	13	A	3.4
3	2D	2	ALA	3.4
40	2i	62	TYR	3.4
29	17	45	ALA	3.3
7	2H	116	GLU	3.3
35	1d	23	GLY	3.3
39	2h	135	CYS	3.3
38	2g	156	TRP	3.3
19	2X	68	ARG	3.3
48	2q	29	HIS	3.3
32	2a	1492	A	3.3
36	2e	109	ILE	3.3
38	2g	83	ALA	3.3
42	1k	60	ALA	3.3
35	2d	68	TYR	3.3
40	2i	7	THR	3.3
17	2V	20	LEU	3.3
7	2H	96	ALA	3.2
39	2h	25	ASP	3.2
44	2m	99	ARG	3.2
40	2i	63	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
8	2I	20	ASP	3.2
22	20	76	GLY	3.2
22	20	52	GLY	3.2
41	2j	7	LYS	3.2
32	2a	1202	G	3.2
55	2z	12	ARG	3.2
6	2G	93	THR	3.2
33	2b	81	VAL	3.2
39	2h	134	ILE	3.2
40	2i	119	ALA	3.2
29	27	47	ARG	3.2
44	2m	121	LYS	3.2
6	2G	94	LEU	3.1
33	2b	97	TRP	3.1
53	2v	21	C	3.1
40	2i	113	LYS	3.1
7	2H	103	LEU	3.1
39	2h	83	ILE	3.1
45	2n	41	ARG	3.1
11	2P	30	THR	3.1
36	1e	119	LEU	3.1
11	2P	34	GLY	3.1
30	18	3	LYS	3.1
40	2i	125	TYR	3.1
6	2G	139	LEU	3.1
8	2I	12	LEU	3.1
33	2b	233	SER	3.1
1	2A	2133	G	3.1
36	1e	92	LYS	3.1
34	2c	160	ALA	3.0
36	2e	94	ALA	3.0
36	2e	33	VAL	3.0
7	2H	114	VAL	3.0
41	1j	59	SER	3.0
3	1D	2	ALA	3.0
9	2N	11	PRO	3.0
38	2g	28	ASN	3.0
51	2t	9	ASN	3.0
55	2z	14	ARG	3.0
6	2G	155	MET	3.0
1	2A	2147	G	3.0
35	2d	99	SER	3.0

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Mol	Chain	Res	Type	RSRZ
44	2m	66	LEU	3.0
41	2j	43	ARG	3.0
11	2P	39	LYS	2.9
7	2H	121	ILE	2.9
6	2G	140	ILE	2.9
45	2n	22	THR	2.9
22	20	75	LEU	2.9
45	2n	36	PHE	2.9
6	2G	41	GLN	2.9
14	2S	35	ILE	2.9
36	2e	65	ASN	2.9
34	2c	23	TYR	2.9
40	1i	115	GLY	2.9
33	2b	214	ILE	2.9
36	2e	11	ILE	2.9
30	28	2	PRO	2.9
53	2v	14	A	2.9
52	2u	10	ARG	2.9
40	2i	36	TYR	2.9
41	2j	64	GLU	2.9
3	2D	215	LEU	2.9
33	2b	77	ALA	2.9
41	2j	63	PHE	2.9
43	2l	69	TYR	2.9
33	2b	29	ALA	2.9
45	2n	53	LEU	2.9
18	2W	85	VAL	2.8
32	1a	1531	A	2.8
53	1v	22	U	2.8
41	2j	10	GLY	2.8
20	2Y	45	VAL	2.8
35	2d	146	ILE	2.8
55	1z	15	TRP	2.8
34	2c	165	THR	2.8
6	2G	89	GLY	2.8
19	2X	92	LEU	2.8
6	2G	102	PHE	2.8
50	2s	34	TRP	2.8
34	2c	184	TYR	2.8
36	2e	141	GLN	2.8
6	2G	35	GLU	2.8
32	2a	1030(B)	C	2.8

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Mol	Chain	Res	Type	RSRZ
49	2r	46	GLU	2.8
16	2U	56	ASP	2.8
39	2h	131	GLY	2.8
51	1t	23	ARG	2.8
33	2b	163	PHE	2.8
22	20	43	THR	2.8
25	23	2	PRO	2.7
40	1i	109	VAL	2.7
31	29	12	ASP	2.7
36	2e	43	LEU	2.7
44	2m	122	LYS	2.7
33	2b	215	LEU	2.7
45	2n	11	LYS	2.7
3	2D	90	ALA	2.7
5	2F	21	ALA	2.7
44	2m	98	VAL	2.7
45	2n	33	VAL	2.7
52	2u	18	TYR	2.7
40	1i	111	ARG	2.7
34	2c	159	GLY	2.7
32	1a	1257	U	2.7
40	2i	115	GLY	2.7
52	2u	14	TRP	2.7
1	2A	859	G	2.7
7	2H	106	THR	2.7
7	2H	89	ILE	2.7
32	2a	506	G	2.7
35	2d	20	TYR	2.7
38	2g	154	TYR	2.7
12	2Q	104	PHE	2.7
22	20	55	ARG	2.7
15	2T	48	ILE	2.7
32	2a	965	A	2.7
38	1g	79	ARG	2.7
27	15	60	VAL	2.7
9	2N	43	THR	2.6
52	2u	23	PRO	2.6
39	2h	113	SER	2.6
33	2b	15	VAL	2.6
30	28	61	LEU	2.6
36	2e	45	PHE	2.6
48	2q	94	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
47	1p	7	ALA	2.6
22	20	80	HIS	2.6
36	1e	82	VAL	2.6
32	2a	788	U	2.6
26	24	40	HIS	2.6
3	2D	204	ILE	2.6
39	2h	112	LEU	2.6
41	2j	8	LEU	2.6
7	2H	102	ALA	2.6
49	2r	43	PHE	2.6
11	2P	35	HIS	2.6
51	1t	21	LYS	2.6
40	2i	13	ALA	2.6
36	2e	29	GLY	2.6
36	2e	130	ASN	2.6
35	1d	138	TYR	2.6
6	2G	34	LEU	2.6
45	1n	49	HIS	2.6
38	2g	27	ILE	2.6
41	2j	47	PHE	2.5
51	1t	9	ASN	2.5
9	2N	9	VAL	2.5
39	2h	101	PRO	2.5
22	20	68	GLU	2.5
22	20	42	GLY	2.5
42	2k	118	GLY	2.5
23	2l	46	LEU	2.5
38	2g	33	ASP	2.5
7	2H	25	LYS	2.5
52	1u	13	ILE	2.5
3	1D	38	LYS	2.5
43	2l	23	LYS	2.5
43	2l	66	VAL	2.5
6	2G	133	LEU	2.5
3	1D	93	ALA	2.5
1	1A	1094	U	2.5
32	2a	1194	U	2.5
42	1k	126	ARG	2.5
45	2n	49	HIS	2.5
53	1v	20	U	2.5
35	2d	75	PHE	2.5
36	1e	101	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
39	2h	91	ARG	2.5
42	2k	25	TYR	2.5
47	1p	15	PRO	2.5
40	2i	33	PHE	2.5
55	1z	14	ARG	2.5
6	2G	135	LEU	2.5
35	2d	2	GLY	2.5
45	2n	44	LEU	2.5
48	2q	37	LYS	2.5
1	2A	1026	U	2.5
22	20	50	ASN	2.5
34	1c	15	THR	2.5
38	1g	85	TYR	2.5
45	1n	59	ALA	2.5
14	2S	87	PHE	2.5
55	1z	13	PRO	2.5
39	1h	2	LEU	2.4
40	2i	41	VAL	2.4
11	2P	21	ARG	2.4
41	2j	60	ARG	2.4
31	29	37	GLY	2.4
41	2j	52	GLY	2.4
11	2P	72	PRO	2.4
45	2n	42	ILE	2.4
35	1d	11	LEU	2.4
41	2j	72	VAL	2.4
17	2V	81	TYR	2.4
20	2Y	35	TYR	2.4
36	2e	81	GLU	2.4
43	2l	67	THR	2.4
9	2N	23	LEU	2.4
34	2c	131	ARG	2.4
6	2G	178	PHE	2.4
11	2P	38	GLN	2.4
20	2Y	43	ASN	2.4
7	2H	145	ALA	2.4
14	2S	37	ALA	2.4
33	2b	79	ASP	2.4
40	2i	117	HIS	2.4
34	2c	4	LYS	2.4
18	1W	111	HIS	2.4
45	2n	59	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
35	2d	202	LEU	2.4
39	1h	119	LEU	2.4
43	1l	91	LYS	2.4
11	2P	15	ARG	2.4
35	2d	70	ILE	2.4
40	2i	32	ASP	2.4
3	1D	37	LEU	2.4
36	2e	79	GLU	2.4
40	2i	110	GLU	2.4
6	2G	28	VAL	2.4
11	2P	101	VAL	2.4
36	2e	105	VAL	2.4
14	2S	57	LYS	2.4
41	1j	64	GLU	2.4
48	1q	28	PRO	2.4
6	2G	40	ASN	2.4
30	28	16	ILE	2.4
34	2c	12	LEU	2.4
45	2n	32	SER	2.3
38	1g	83	ALA	2.3
6	2G	19	LEU	2.3
30	28	50	LEU	2.3
17	2V	17	GLY	2.3
33	2b	93	VAL	2.3
20	1Y	1	MET	2.3
1	1A	1096	A	2.3
7	2H	105	LEU	2.3
17	2V	42	GLY	2.3
26	14	49	PHE	2.3
35	2d	23	GLY	2.3
48	2q	27	PHE	2.3
35	2d	152	SER	2.3
43	2l	68	ALA	2.3
1	2A	229	A	2.3
34	2c	204	LEU	2.3
18	2W	78	GLU	2.3
30	28	24	ALA	2.3
45	2n	7	ILE	2.3
20	2Y	42	VAL	2.3
40	2i	67	GLY	2.3
41	2j	70	ARG	2.3
51	2t	80	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
17	2V	76	LYS	2.3
45	1n	56	VAL	2.3
52	2u	11	GLY	2.3
30	28	12	LYS	2.3
34	1c	154	SER	2.3
44	2m	101	GLN	2.3
19	2X	69	TYR	2.3
7	2H	101	ARG	2.3
32	2a	1343	G	2.3
41	2j	97	GLU	2.3
33	2b	48	MET	2.3
39	2h	2	LEU	2.3
39	2h	133	LEU	2.3
40	1i	126	SER	2.3
6	2G	157	ILE	2.3
7	2H	141	VAL	2.3
30	28	23	VAL	2.3
52	1u	16	GLY	2.3
1	2A	2170	A	2.3
18	2W	82	LEU	2.3
20	2Y	32	PRO	2.3
41	2j	96	ILE	2.3
1	1A	1026	U	2.3
18	2W	94	ASP	2.3
52	2u	8	THR	2.3
33	2b	131	PRO	2.3
6	2G	75	LYS	2.3
53	1v	13	A	2.3
33	2b	195	ASP	2.2
22	20	38	VAL	2.2
34	2c	189	ALA	2.2
3	2D	219	PRO	2.2
30	28	63	PRO	2.2
14	2S	45	GLY	2.2
34	1c	2	GLY	2.2
40	2i	114	TYR	2.2
5	2F	65	TRP	2.2
19	1X	60	ARG	2.2
34	2c	167	TRP	2.2
6	2G	90	LEU	2.2
20	2Y	44	ILE	2.2
3	1D	55	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
6	2G	80	PHE	2.2
39	2h	95	VAL	2.2
43	1l	61	THR	2.2
50	2s	15	LEU	2.2
5	2F	78	ILE	2.2
5	2F	82	ILE	2.2
14	2S	85	VAL	2.2
36	2e	82	VAL	2.2
3	2D	38	LYS	2.2
6	2G	74	LYS	2.2
18	2W	97	LYS	2.2
3	2D	156	ALA	2.2
33	2b	67	THR	2.2
42	2k	123	LYS	2.2
1	2A	2142	C	2.2
20	2Y	62	GLU	2.2
23	2l	34	THR	2.2
36	2e	119	LEU	2.2
30	28	59	LYS	2.2
39	1h	80	ILE	2.2
26	24	34	GLU	2.2
51	1t	19	SER	2.2
32	2a	1114	C	2.2
51	2t	26	ASN	2.2
39	2h	109	ILE	2.2
41	2j	68	HIS	2.2
46	2o	45	VAL	2.2
34	1c	189	ALA	2.2
45	2n	2	ALA	2.2
22	20	77	ARG	2.2
45	2n	50	LYS	2.2
51	1t	18	GLN	2.2
10	2O	1	MET	2.2
35	2d	158	ILE	2.2
11	2P	68	GLN	2.2
35	2d	150	GLU	2.2
36	2e	115	VAL	2.2
18	2W	38	TYR	2.2
28	26	10	LEU	2.2
25	23	12	PRO	2.2
32	2a	1187	G	2.2
33	2b	28	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
34	2c	180	ALA	2.1
40	2i	4	TYR	2.1
9	2N	50	ASP	2.1
38	1g	80	VAL	2.1
1	2A	2446	G	2.1
22	20	54	GLY	2.1
34	2c	6	HIS	2.1
33	2b	146	GLN	2.1
6	2G	33	ARG	2.1
17	2V	19	LYS	2.1
35	2d	69	GLY	2.1
24	22	24	LEU	2.1
5	2F	51	THR	2.1
38	1g	153	HIS	2.1
33	2b	68	ILE	2.1
35	1d	24	GLU	2.1
38	2g	85	TYR	2.1
29	27	23	ARG	2.1
39	2h	92	ARG	2.1
41	2j	54	PHE	2.1
40	2i	14	VAL	2.1
6	2G	32	PRO	2.1
40	2i	68	GLY	2.1
1	2A	2132	U	2.1
3	2D	59	LYS	2.1
34	1c	169	ALA	2.1
27	25	11	THR	2.1
48	1q	26	GLN	2.1
7	2H	138	LYS	2.1
42	1k	25	TYR	2.1
32	2a	1030(A)	G	2.1
6	2G	92	VAL	2.1
12	1Q	80	GLU	2.1
12	2Q	80	GLU	2.1
26	24	53	GLU	2.1
52	2u	17	THR	2.1
40	2i	127	LYS	2.1
39	2h	86	ILE	2.1
1	1A	435	C	2.1
41	2j	5	ARG	2.1
20	2Y	60	PHE	2.1
9	1N	72	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
33	2b	41	ILE	2.1
40	2i	116	LYS	2.1
6	2G	112	PRO	2.1
30	18	53	PRO	2.1
9	2N	47	ALA	2.1
36	1e	86	ALA	2.1
47	1p	38	TYR	2.1
23	2l	62	VAL	2.1
47	2p	19	ILE	2.1
30	28	62	LEU	2.1
43	2l	60	LEU	2.1
22	20	45	PHE	2.1
36	2e	90	VAL	2.1
43	1l	89	ARG	2.1
3	2D	231	HIS	2.1
23	2l	66	HIS	2.1
22	20	74	ARG	2.1
35	2d	122	ARG	2.1
41	2j	55	LYS	2.1
33	2b	92	TYR	2.1
40	2i	70	LYS	2.0
51	1t	17	ARG	2.0
1	1A	614(B)	G	2.0
7	2H	94	TYR	2.0
32	2a	1224	G	2.0
26	24	35	VAL	2.0
26	24	56	VAL	2.0
39	2h	137	VAL	2.0
8	2l	35	LEU	2.0
1	1A	1762	A	2.0
21	2Z	88	PHE	2.0
33	2b	152	PHE	2.0
36	1e	28	PHE	2.0
38	2g	84	ASN	2.0
1	1A	2132	U	2.0
38	2g	9	VAL	2.0
40	2i	109	VAL	2.0
34	1c	188	LEU	2.0
22	20	71	ASP	2.0
38	2g	38	LEU	2.0
7	2H	82	GLY	2.0
1	2A	34	C	2.0

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Mol	Chain	Res	Type	RSRZ
12	2Q	99	PRO	2.0
18	2W	81	ALA	2.0
25	23	30	ARG	2.0
28	26	2	ALA	2.0
40	2i	66	ARG	2.0
44	2m	96	LEU	2.0
45	2n	6	LEU	2.0
1	1A	2141	G	2.0
33	1b	202	PRO	2.0
3	1D	40	THR	2.0
40	2i	121	ARG	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
54	4SU	2x	8	20/21	0.88	0.15	77,86,93,93	0
54	PSU	2x	55	20/21	0.90	0.11	75,83,93,101	0
32	4OC	2a	1402	22/23	0.91	0.22	64,69,76,79	0
32	PSU	2a	516	20/21	0.91	0.19	66,74,81,82	0
32	5MC	2a	1400	21/22	0.92	0.21	56,70,78,81	0
32	5MC	2a	967	21/22	0.92	0.27	67,72,81,85	0
32	2MG	2a	1207	24/25	0.93	0.17	76,83,88,95	0
32	M2G	2a	966	25/26	0.93	0.24	64,71,81,85	0
32	5MC	2a	1404	21/22	0.93	0.19	56,64,71,74	0
1	5MU	2A	1915	21/22	0.93	0.14	74,78,84,97	0
1	4OC	2A	1920	21/23	0.93	0.27	55,64,71,78	0
54	5MC	2x	32	21/22	0.93	0.22	68,74,76,78	0
32	7MG	2a	527	24/25	0.94	0.20	65,69,75,76	0
54	5MU	2x	54	21/22	0.94	0.14	79,82,89,97	0
1	PSU	2A	1911	20/21	0.94	0.18	64,69,77,77	0
32	MA6	2a	1519	24/25	0.94	0.32	54,61,67,73	0
32	2MG	1a	1207	24/25	0.94	0.17	54,66,75,81	0
43	0TD	2l	92	10/11	0.94	0.24	57,62,66,79	0
1	5MC	2A	1962	21/22	0.95	0.18	45,55,59,64	0
1	PSU	2A	1917	20/21	0.95	0.15	58,69,74,76	0
32	4OC	1a	1402	22/23	0.95	0.24	48,54,61,63	0
32	MA6	2a	1518	24/25	0.95	0.28	53,63,68,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	4SU	1x	8	20/21	0.95	0.14	60,67,74,76	0
54	PSU	1x	55	20/21	0.95	0.14	62,65,72,76	0
1	5MC	2A	1942	21/22	0.95	0.17	49,62,66,67	0
54	5MU	1x	54	21/22	0.96	0.13	60,66,70,74	0
32	5MC	1a	1404	21/22	0.96	0.23	40,50,54,56	0
1	PSU	1A	1911	20/21	0.96	0.18	46,57,61,64	0
1	5MC	1A	1942	21/22	0.96	0.20	39,45,50,58	0
54	5MC	1x	32	21/22	0.96	0.23	47,53,58,64	0
32	M2G	1a	966	25/26	0.96	0.24	54,58,61,66	0
1	5MU	1A	1915	21/22	0.96	0.17	52,64,73,80	0
1	PSU	1A	1917	20/21	0.96	0.16	55,61,66,68	0
32	7MG	1a	527	24/25	0.96	0.18	40,50,56,60	0
43	0TD	1l	92	10/11	0.96	0.21	53,56,59,62	0
32	PSU	1a	516	20/21	0.96	0.17	54,64,68,71	0
32	UR3	2a	1498	21/22	0.96	0.30	46,54,62,69	0
32	5MC	1a	967	21/22	0.96	0.25	55,63,65,65	0
32	UR3	1a	1498	21/22	0.97	0.22	42,49,56,60	0
1	4OC	1A	1920	21/23	0.97	0.23	39,52,55,65	0
1	2MA	2A	2503	23/24	0.97	0.25	39,46,49,52	0
1	OMG	2A	2251	24/25	0.97	0.23	35,44,49,50	0
1	PSU	2A	2605	20/21	0.97	0.21	35,42,46,46	0
1	5MU	2A	1939	21/22	0.97	0.18	32,48,52,55	0
32	5MC	2a	1407	21/22	0.97	0.23	49,61,69,71	0
32	5MC	1a	1400	21/22	0.97	0.19	49,55,62,70	0
32	MA6	1a	1518	24/25	0.97	0.24	34,49,55,55	0
1	OMG	1A	2251	24/25	0.97	0.25	26,37,40,44	0
1	5MC	1A	1962	21/22	0.97	0.25	35,44,48,50	0
1	2MU	1A	2552	21/23	0.98	0.22	26,37,42,48	0
32	5MC	1a	1407	21/22	0.98	0.20	39,45,49,51	0
1	PSU	1A	2605	20/21	0.98	0.24	28,36,41,42	0
1	2MU	2A	2552	21/23	0.98	0.20	33,42,49,52	0
32	MA6	1a	1519	24/25	0.98	0.27	44,52,54,55	0
1	2MA	1A	2503	23/24	0.98	0.23	24,32,35,41	0
1	5MU	1A	1939	21/22	0.98	0.26	28,36,41,43	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	1A	3407	1/1	0.31	0.52	103,103,103,103	0
56	MG	2A	3351	1/1	0.48	0.26	59,59,59,59	0
56	MG	2A	3206	1/1	0.60	0.16	52,52,52,52	0
56	MG	2a	3105	1/1	0.60	0.30	53,53,53,53	0
56	MG	1A	3399	1/1	0.63	0.29	70,70,70,70	0
56	MG	2a	3119	1/1	0.63	0.40	76,76,76,76	0
56	MG	2A	3337	1/1	0.64	0.22	56,56,56,56	0
56	MG	1A	3151	1/1	0.64	0.43	72,72,72,72	0
56	MG	2A	3229	1/1	0.64	0.30	56,56,56,56	0
56	MG	1A	3373	1/1	0.65	0.34	47,47,47,47	0
56	MG	2a	3023	1/1	0.66	0.26	59,59,59,59	0
56	MG	1A	3575	1/1	0.67	0.21	72,72,72,72	0
56	MG	2a	3082	1/1	0.67	0.22	61,61,61,61	0
57	ZN	24	501	1/1	0.67	0.06	130,130,130,130	0
56	MG	2A	3515	1/1	0.68	0.15	39,39,39,39	0
56	MG	2A	3126	1/1	0.69	0.16	51,51,51,51	0
56	MG	2a	3024	1/1	0.69	0.24	59,59,59,59	0
56	MG	1A	3773	1/1	0.69	0.13	69,69,69,69	0
56	MG	2A	3197	1/1	0.69	0.22	73,73,73,73	0
56	MG	2a	3057	1/1	0.71	0.19	59,59,59,59	0
56	MG	1A	3239	1/1	0.71	0.23	53,53,53,53	0
56	MG	1A	3212	1/1	0.71	0.28	45,45,45,45	0
56	MG	1A	3150	1/1	0.72	0.52	35,35,35,35	0
56	MG	2r	101	1/1	0.72	0.13	65,65,65,65	0
56	MG	2v	101	1/1	0.73	0.40	77,77,77,77	0
56	MG	2A	3280	1/1	0.73	0.19	49,49,49,49	0
56	MG	1A	3187	1/1	0.74	0.19	49,49,49,49	0
56	MG	1A	3233	1/1	0.74	0.15	62,62,62,62	0
56	MG	2a	3048	1/1	0.75	0.28	61,61,61,61	0
56	MG	2A	3516	1/1	0.75	0.22	67,67,67,67	0
56	MG	2A	3186	1/1	0.76	0.22	52,52,52,52	0
56	MG	1a	1621	1/1	0.76	0.19	51,51,51,51	0
56	MG	2A	3155	1/1	0.76	0.30	61,61,61,61	0
56	MG	1A	3488	1/1	0.77	0.09	47,47,47,47	0
56	MG	1A	3618	1/1	0.77	0.18	23,23,23,23	0
56	MG	1A	3480	1/1	0.77	0.17	28,28,28,28	0
56	MG	1A	3152	1/1	0.77	0.89	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1B	213	1/1	0.77	0.29	58,58,58,58	0
56	MG	1A	3179	1/1	0.77	0.14	59,59,59,59	0
56	MG	1a	1681	1/1	0.77	0.24	55,55,55,55	0
56	MG	2A	3366	1/1	0.78	0.28	53,53,53,53	0
56	MG	2a	3121	1/1	0.78	0.19	48,48,48,48	0
56	MG	2a	3095	1/1	0.78	0.17	57,57,57,57	0
56	MG	2A	3262	1/1	0.78	0.28	46,46,46,46	0
56	MG	2A	3274	1/1	0.78	0.13	51,51,51,51	0
56	MG	2A	3167	1/1	0.78	0.24	61,61,61,61	0
56	MG	1A	3763	1/1	0.78	0.28	68,68,68,68	0
56	MG	2A	3254	1/1	0.79	0.58	40,40,40,40	0
56	MG	1E	305	1/1	0.79	0.40	52,52,52,52	0
56	MG	2B	201	1/1	0.79	0.22	67,67,67,67	0
56	MG	1A	3230	1/1	0.79	0.37	49,49,49,49	0
56	MG	1A	3439	1/1	0.79	0.17	50,50,50,50	0
56	MG	2A	3312	1/1	0.79	0.43	53,53,53,53	0
56	MG	2A	3308	1/1	0.79	0.12	55,55,55,55	0
56	MG	1A	3631	1/1	0.79	0.08	69,69,69,69	0
56	MG	1a	1644	1/1	0.79	0.18	54,54,54,54	0
56	MG	2A	3026	1/1	0.79	0.22	60,60,60,60	0
56	MG	2A	3010	1/1	0.79	0.38	56,56,56,56	0
56	MG	2A	3152	1/1	0.79	0.21	64,64,64,64	0
56	MG	1A	3522	1/1	0.79	0.14	26,26,26,26	0
56	MG	1A	3243	1/1	0.79	0.22	46,46,46,46	0
56	MG	2A	3483	1/1	0.80	0.17	73,73,73,73	0
56	MG	2A	3354	1/1	0.80	0.16	46,46,46,46	0
56	MG	2A	3067	1/1	0.80	0.22	55,55,55,55	0
56	MG	1A	3059	1/1	0.80	0.25	58,58,58,58	0
56	MG	1A	3710	1/1	0.80	0.14	50,50,50,50	0
56	MG	2A	3467	1/1	0.80	0.09	33,33,33,33	0
56	MG	1A	3267	1/1	0.80	0.29	61,61,61,61	0
56	MG	2A	3330	1/1	0.80	0.18	50,50,50,50	0
56	MG	2A	3421	1/1	0.80	0.30	54,54,54,54	0
56	MG	2A	3065	1/1	0.80	0.16	57,57,57,57	0
56	MG	2A	3048	1/1	0.80	0.17	58,58,58,58	0
56	MG	2A	3368	1/1	0.80	0.23	70,70,70,70	0
56	MG	1a	1742	1/1	0.81	0.21	60,60,60,60	0
56	MG	1A	3051	1/1	0.81	0.15	43,43,43,43	0
56	MG	2A	3439	1/1	0.81	0.27	47,47,47,47	0
56	MG	1A	3390	1/1	0.81	0.88	50,50,50,50	0
56	MG	2a	3139	1/1	0.81	0.16	54,54,54,54	0
56	MG	1A	3784	1/1	0.81	0.46	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3463	1/1	0.81	0.14	44,44,44,44	0
56	MG	1A	3039	1/1	0.81	0.66	44,44,44,44	0
56	MG	2A	3011	1/1	0.81	0.50	28,28,28,28	0
56	MG	1B	204	1/1	0.81	0.16	38,38,38,38	0
56	MG	2a	3140	1/1	0.81	0.21	64,64,64,64	0
56	MG	26	101	1/1	0.81	0.40	56,56,56,56	0
56	MG	1A	3774	1/1	0.81	0.42	80,80,80,80	0
56	MG	2A	3063	1/1	0.81	0.14	46,46,46,46	0
56	MG	1a	1723	1/1	0.81	0.13	57,57,57,57	0
56	MG	2A	3340	1/1	0.81	0.26	60,60,60,60	0
56	MG	2A	3253	1/1	0.81	0.12	63,63,63,63	0
56	MG	2A	3326	1/1	0.81	0.15	62,62,62,62	0
56	MG	2A	3512	1/1	0.81	0.11	39,39,39,39	0
56	MG	1A	3210	1/1	0.81	0.21	48,48,48,48	0
56	MG	1A	3767	1/1	0.82	0.21	51,51,51,51	0
56	MG	1A	3753	1/1	0.82	0.22	31,31,31,31	0
56	MG	1A	3772	1/1	0.82	0.15	59,59,59,59	0
56	MG	1a	1744	1/1	0.82	0.20	58,58,58,58	0
56	MG	2A	3387	1/1	0.82	0.18	38,38,38,38	0
56	MG	1A	3455	1/1	0.82	0.18	50,50,50,50	0
56	MG	1A	3837	1/1	0.82	0.24	64,64,64,64	0
56	MG	1A	3297	1/1	0.82	0.45	55,55,55,55	0
56	MG	2a	3133	1/1	0.82	0.18	55,55,55,55	0
56	MG	1A	3284	1/1	0.82	0.17	51,51,51,51	0
56	MG	1A	3396	1/1	0.82	0.24	43,43,43,43	0
56	MG	1a	1706	1/1	0.82	0.16	48,48,48,48	0
56	MG	2A	3180	1/1	0.82	0.23	48,48,48,48	0
56	MG	1G	202	1/1	0.82	0.23	37,37,37,37	0
56	MG	2j	201	1/1	0.82	0.13	58,58,58,58	0
56	MG	2A	3339	1/1	0.82	0.13	63,63,63,63	0
56	MG	2A	3317	1/1	0.82	0.11	59,59,59,59	0
56	MG	1A	3687	1/1	0.82	0.18	58,58,58,58	0
56	MG	2A	3051	1/1	0.82	0.15	54,54,54,54	0
56	MG	1A	3557	1/1	0.82	0.17	43,43,43,43	0
56	MG	1X	103	1/1	0.82	0.48	40,40,40,40	0
56	MG	1A	3338	1/1	0.82	0.52	39,39,39,39	0
56	MG	1a	1719	1/1	0.82	0.37	53,53,53,53	0
56	MG	1A	3358	1/1	0.82	0.22	54,54,54,54	0
56	MG	1A	3663	1/1	0.83	0.62	41,41,41,41	0
56	MG	2A	3394	1/1	0.83	0.20	60,60,60,60	0
56	MG	1A	3802	1/1	0.83	0.21	37,37,37,37	0
56	MG	2F	302	1/1	0.83	0.58	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3257	1/1	0.83	0.31	52,52,52,52	0
56	MG	2A	3506	1/1	0.83	0.19	68,68,68,68	0
56	MG	1A	3172	1/1	0.83	0.20	52,52,52,52	0
56	MG	1A	3497	1/1	0.83	0.16	45,45,45,45	0
56	MG	2a	3110	1/1	0.83	0.19	60,60,60,60	0
56	MG	2A	3344	1/1	0.83	0.17	66,66,66,66	0
56	MG	2a	3039	1/1	0.83	0.08	58,58,58,58	0
56	MG	1A	3475	1/1	0.83	0.13	29,29,29,29	0
56	MG	1A	3024	1/1	0.83	0.08	76,76,76,76	0
56	MG	1a	1680	1/1	0.83	0.25	60,60,60,60	0
56	MG	2a	3055	1/1	0.83	0.11	61,61,61,61	0
56	MG	1a	1764	1/1	0.83	0.08	52,52,52,52	0
56	MG	2A	3486	1/1	0.83	0.15	41,41,41,41	0
56	MG	2A	3355	1/1	0.83	0.41	61,61,61,61	0
56	MG	2a	3112	1/1	0.83	0.16	64,64,64,64	0
56	MG	1a	1724	1/1	0.83	0.13	52,52,52,52	0
56	MG	1A	3146	1/1	0.83	0.26	40,40,40,40	0
56	MG	1A	3595	1/1	0.83	0.14	56,56,56,56	0
56	MG	1F	305	1/1	0.83	0.21	40,40,40,40	0
56	MG	2N	201	1/1	0.83	0.16	49,49,49,49	0
56	MG	1a	1615	1/1	0.83	0.14	52,52,52,52	0
56	MG	2A	3335	1/1	0.83	0.20	58,58,58,58	0
56	MG	1A	3165	1/1	0.84	0.10	29,29,29,29	0
56	MG	2a	3132	1/1	0.84	0.36	55,55,55,55	0
56	MG	1A	3303	1/1	0.84	0.25	58,58,58,58	0
56	MG	1A	3602	1/1	0.84	0.08	56,56,56,56	0
56	MG	14	101	1/1	0.84	0.24	56,56,56,56	0
56	MG	2a	3086	1/1	0.84	0.31	69,69,69,69	0
56	MG	2a	3116	1/1	0.84	0.16	51,51,51,51	0
56	MG	1A	3244	1/1	0.84	0.19	49,49,49,49	0
56	MG	1A	3796	1/1	0.84	0.11	69,69,69,69	0
56	MG	2a	3054	1/1	0.84	0.16	63,63,63,63	0
56	MG	1A	3627	1/1	0.84	0.12	36,36,36,36	0
56	MG	2a	3028	1/1	0.84	0.13	49,49,49,49	0
56	MG	1A	3301	1/1	0.84	0.71	33,33,33,33	0
56	MG	1A	3273	1/1	0.84	0.46	59,59,59,59	0
56	MG	1a	1728	1/1	0.84	0.22	63,63,63,63	0
56	MG	1a	1639	1/1	0.84	0.18	40,40,40,40	0
56	MG	1a	1663	1/1	0.84	0.20	53,53,53,53	0
56	MG	2A	3361	1/1	0.84	0.13	49,49,49,49	0
56	MG	1A	3384	1/1	0.84	0.15	41,41,41,41	0
56	MG	1A	3785	1/1	0.84	0.12	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3369	1/1	0.84	0.22	42,42,42,42	0
56	MG	2A	3376	1/1	0.84	0.33	52,52,52,52	0
56	MG	2a	3135	1/1	0.84	0.11	64,64,64,64	0
56	MG	2A	3370	1/1	0.84	0.15	51,51,51,51	0
56	MG	17	3105	1/1	0.84	0.18	28,28,28,28	0
56	MG	2a	3084	1/1	0.84	0.22	67,67,67,67	0
56	MG	2A	3122	1/1	0.84	0.13	54,54,54,54	0
56	MG	1A	3754	1/1	0.84	0.14	61,61,61,61	0
56	MG	1A	3826	1/1	0.84	0.22	51,51,51,51	0
56	MG	1A	3697	1/1	0.84	0.20	25,25,25,25	0
56	MG	2A	3484	1/1	0.84	0.09	44,44,44,44	0
56	MG	1A	3286	1/1	0.85	0.29	39,39,39,39	0
56	MG	1a	1675	1/1	0.85	0.24	53,53,53,53	0
56	MG	1A	3345	1/1	0.85	0.15	50,50,50,50	0
56	MG	1A	3072	1/1	0.85	0.23	52,52,52,52	0
56	MG	1A	3014	1/1	0.85	0.17	24,24,24,24	0
56	MG	1a	1686	1/1	0.85	0.34	64,64,64,64	0
56	MG	19	101	1/1	0.85	0.23	52,52,52,52	0
56	MG	2x	102	1/1	0.85	0.22	47,47,47,47	0
56	MG	2A	3096	1/1	0.85	0.15	49,49,49,49	0
56	MG	1A	3079	1/1	0.85	0.14	32,32,32,32	0
56	MG	23	101	1/1	0.85	0.56	45,45,45,45	0
56	MG	2A	3625	1/1	0.85	0.18	51,51,51,51	0
56	MG	2A	3471	1/1	0.85	0.12	54,54,54,54	0
56	MG	1A	3019	1/1	0.85	0.26	39,39,39,39	0
56	MG	2a	3062	1/1	0.85	0.18	62,62,62,62	0
56	MG	2v	102	1/1	0.85	0.25	57,57,57,57	0
56	MG	1A	3271	1/1	0.85	0.14	47,47,47,47	0
56	MG	2A	3025	1/1	0.85	0.44	53,53,53,53	0
56	MG	1f	202	1/1	0.85	0.18	54,54,54,54	0
56	MG	2a	3079	1/1	0.85	0.25	52,52,52,52	0
56	MG	1A	3125	1/1	0.85	0.19	49,49,49,49	0
56	MG	1Z	301	1/1	0.85	0.26	41,41,41,41	0
56	MG	2A	3299	1/1	0.85	0.17	46,46,46,46	0
56	MG	1A	3289	1/1	0.85	0.12	46,46,46,46	0
56	MG	2A	3550	1/1	0.85	0.25	61,61,61,61	0
56	MG	2A	3310	1/1	0.85	0.23	44,44,44,44	0
56	MG	2A	3409	1/1	0.85	0.19	60,60,60,60	0
56	MG	2a	3006	1/1	0.85	0.11	63,63,63,63	0
56	MG	1A	3217	1/1	0.85	0.24	53,53,53,53	0
56	MG	1A	3320	1/1	0.85	0.18	59,59,59,59	0
56	MG	1A	3177	1/1	0.85	0.20	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3026	1/1	0.85	0.22	45,45,45,45	0
56	MG	1A	3313	1/1	0.85	0.54	34,34,34,34	0
56	MG	1A	3715	1/1	0.85	0.15	53,53,53,53	0
56	MG	2A	3566	1/1	0.85	0.14	62,62,62,62	0
56	MG	2E	301	1/1	0.85	0.17	42,42,42,42	0
56	MG	1s	101	1/1	0.85	0.25	55,55,55,55	0
56	MG	1a	1717	1/1	0.85	0.25	67,67,67,67	0
56	MG	1A	3071	1/1	0.86	0.22	38,38,38,38	0
56	MG	2a	3094	1/1	0.86	0.17	57,57,57,57	0
56	MG	2A	3123	1/1	0.86	0.26	51,51,51,51	0
56	MG	2A	3225	1/1	0.86	0.17	51,51,51,51	0
56	MG	2P	202	1/1	0.86	0.24	34,34,34,34	0
56	MG	1a	1737	1/1	0.86	0.17	41,41,41,41	0
56	MG	1A	3274	1/1	0.86	0.17	52,52,52,52	0
56	MG	2a	3064	1/1	0.86	0.15	64,64,64,64	0
56	MG	2A	3416	1/1	0.86	0.20	63,63,63,63	0
56	MG	1A	3260	1/1	0.86	0.19	48,48,48,48	0
56	MG	1A	3307	1/1	0.86	0.63	52,52,52,52	0
56	MG	2A	3016	1/1	0.86	0.32	65,65,65,65	0
56	MG	1A	3572	1/1	0.86	0.52	71,71,71,71	0
56	MG	1A	3232	1/1	0.86	0.54	46,46,46,46	0
56	MG	2A	3315	1/1	0.86	0.18	51,51,51,51	0
56	MG	2a	3025	1/1	0.86	0.11	73,73,73,73	0
56	MG	1A	3149	1/1	0.86	0.78	58,58,58,58	0
56	MG	2a	3038	1/1	0.86	0.12	52,52,52,52	0
56	MG	1A	3124	1/1	0.86	0.48	46,46,46,46	0
56	MG	2A	3146	1/1	0.86	0.13	42,42,42,42	0
56	MG	2A	3085	1/1	0.86	0.17	42,42,42,42	0
56	MG	2a	3036	1/1	0.86	0.10	58,58,58,58	0
56	MG	2A	3325	1/1	0.86	0.27	52,52,52,52	0
56	MG	1A	3540	1/1	0.86	0.17	28,28,28,28	0
56	MG	1A	3107	1/1	0.86	0.52	29,29,29,29	0
56	MG	1a	1634	1/1	0.86	0.22	49,49,49,49	0
56	MG	1A	3007	1/1	0.86	0.32	54,54,54,54	0
56	MG	1a	1739	1/1	0.86	0.13	48,48,48,48	0
56	MG	1A	3648	1/1	0.86	0.14	62,62,62,62	0
56	MG	1A	3160	1/1	0.86	0.20	34,34,34,34	0
56	MG	2A	3217	1/1	0.86	0.14	48,48,48,48	0
56	MG	1A	3403	1/1	0.86	0.19	56,56,56,56	0
56	MG	1A	3543	1/1	0.86	0.20	29,29,29,29	0
56	MG	2a	3124	1/1	0.86	0.15	56,56,56,56	0
56	MG	1A	3371	1/1	0.86	0.27	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2a	3120	1/1	0.86	0.23	37,37,37,37	0
56	MG	2A	3369	1/1	0.86	0.32	58,58,58,58	0
56	MG	2A	3591	1/1	0.86	0.15	36,36,36,36	0
56	MG	1A	3667	1/1	0.86	0.18	33,33,33,33	0
56	MG	2A	3346	1/1	0.86	0.17	45,45,45,45	0
56	MG	1A	3129	1/1	0.86	0.09	45,45,45,45	0
56	MG	1A	3414	1/1	0.86	0.14	40,40,40,40	0
56	MG	1A	3679	1/1	0.86	0.13	52,52,52,52	0
56	MG	1A	3352	1/1	0.87	0.25	48,48,48,48	0
56	MG	2t	201	1/1	0.87	0.20	49,49,49,49	0
56	MG	2a	3089	1/1	0.87	0.24	57,57,57,57	0
56	MG	2A	3173	1/1	0.87	0.17	47,47,47,47	0
56	MG	2A	3082	1/1	0.87	0.13	52,52,52,52	0
56	MG	1a	1759	1/1	0.87	0.17	65,65,65,65	0
56	MG	2A	3399	1/1	0.87	0.17	47,47,47,47	0
56	MG	1a	1745	1/1	0.87	0.28	44,44,44,44	0
56	MG	1a	1709	1/1	0.87	0.18	36,36,36,36	0
56	MG	2A	3147	1/1	0.87	0.28	59,59,59,59	0
56	MG	1x	106	1/1	0.87	0.20	72,72,72,72	0
56	MG	1A	3848	1/1	0.87	0.23	46,46,46,46	0
56	MG	1A	3382	1/1	0.87	0.17	57,57,57,57	0
56	MG	2A	3333	1/1	0.87	0.12	51,51,51,51	0
56	MG	1A	3520	1/1	0.87	0.16	37,37,37,37	0
56	MG	1A	3073	1/1	0.87	0.18	30,30,30,30	0
56	MG	2V	202	1/1	0.87	0.51	53,53,53,53	0
56	MG	2A	3428	1/1	0.87	0.29	50,50,50,50	0
56	MG	2a	3106	1/1	0.87	0.10	60,60,60,60	0
56	MG	2a	3003	1/1	0.87	0.16	61,61,61,61	0
56	MG	2A	3250	1/1	0.87	0.20	38,38,38,38	0
56	MG	1B	215	1/1	0.87	0.32	44,44,44,44	0
56	MG	1N	203	1/1	0.87	0.12	31,31,31,31	0
56	MG	2B	206	1/1	0.87	0.19	64,64,64,64	0
56	MG	1A	3795	1/1	0.87	0.10	39,39,39,39	0
56	MG	1A	3074	1/1	0.87	0.17	55,55,55,55	0
56	MG	1A	3171	1/1	0.87	0.16	49,49,49,49	0
56	MG	2a	3090	1/1	0.87	0.24	52,52,52,52	0
56	MG	2A	3318	1/1	0.87	0.28	51,51,51,51	0
56	MG	2A	3323	1/1	0.87	0.16	50,50,50,50	0
56	MG	1A	3173	1/1	0.87	0.14	52,52,52,52	0
56	MG	1A	3353	1/1	0.87	0.17	49,49,49,49	0
56	MG	1A	3248	1/1	0.87	0.39	49,49,49,49	0
56	MG	1A	3216	1/1	0.87	0.16	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3841	1/1	0.87	0.26	57,57,57,57	0
56	MG	1B	205	1/1	0.87	0.21	53,53,53,53	0
56	MG	1A	3250	1/1	0.87	0.69	30,30,30,30	0
56	MG	2A	3151	1/1	0.87	0.26	53,53,53,53	0
56	MG	2A	3195	1/1	0.87	0.22	50,50,50,50	0
56	MG	2A	3219	1/1	0.87	0.19	47,47,47,47	0
56	MG	1A	3805	1/1	0.87	0.11	54,54,54,54	0
56	MG	2a	3021	1/1	0.87	0.27	68,68,68,68	0
56	MG	2A	3442	1/1	0.87	0.26	54,54,54,54	0
56	MG	1a	1623	1/1	0.87	0.12	56,56,56,56	0
56	MG	1A	3768	1/1	0.87	0.08	52,52,52,52	0
56	MG	2a	3018	1/1	0.87	0.12	59,59,59,59	0
56	MG	2A	3372	1/1	0.88	0.46	62,62,62,62	0
56	MG	1x	102	1/1	0.88	0.19	45,45,45,45	0
56	MG	2a	3072	1/1	0.88	0.10	55,55,55,55	0
56	MG	1A	3300	1/1	0.88	0.23	30,30,30,30	0
56	MG	1U	205	1/1	0.88	0.15	39,39,39,39	0
56	MG	2A	3341	1/1	0.88	0.29	56,56,56,56	0
56	MG	12	101	1/1	0.88	0.29	37,37,37,37	0
56	MG	1A	3226	1/1	0.88	0.14	47,47,47,47	0
56	MG	2A	3261	1/1	0.88	0.38	53,53,53,53	0
56	MG	1A	3285	1/1	0.88	0.40	35,35,35,35	0
56	MG	1A	3395	1/1	0.88	0.12	45,45,45,45	0
56	MG	2A	3083	1/1	0.88	0.09	49,49,49,49	0
56	MG	1A	3617	1/1	0.88	0.33	48,48,48,48	0
56	MG	1A	3551	1/1	0.88	0.14	30,30,30,30	0
56	MG	2A	3245	1/1	0.88	0.08	46,46,46,46	0
56	MG	2A	3259	1/1	0.88	0.33	40,40,40,40	0
56	MG	2a	3033	1/1	0.88	0.14	57,57,57,57	0
56	MG	1A	3737	1/1	0.88	0.15	47,47,47,47	0
56	MG	2a	3096	1/1	0.88	0.25	58,58,58,58	0
56	MG	1a	1628	1/1	0.88	0.15	43,43,43,43	0
56	MG	2a	3081	1/1	0.88	0.20	55,55,55,55	0
56	MG	1A	3786	1/1	0.88	0.30	58,58,58,58	0
56	MG	1A	3278	1/1	0.88	0.36	46,46,46,46	0
56	MG	2A	3375	1/1	0.88	0.29	51,51,51,51	0
56	MG	1A	3270	1/1	0.88	0.12	50,50,50,50	0
56	MG	2A	3356	1/1	0.88	0.14	61,61,61,61	0
56	MG	2a	3109	1/1	0.88	0.12	60,60,60,60	0
56	MG	1x	110	1/1	0.88	0.34	53,53,53,53	0
56	MG	2a	3020	1/1	0.88	0.14	49,49,49,49	0
56	MG	2a	3009	1/1	0.88	0.36	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3383	1/1	0.88	0.23	69,69,69,69	0
56	MG	1a	1627	1/1	0.88	0.16	60,60,60,60	0
56	MG	2A	3294	1/1	0.88	0.13	51,51,51,51	0
56	MG	2a	3126	1/1	0.88	0.16	66,66,66,66	0
56	MG	2a	3001	1/1	0.88	0.18	55,55,55,55	0
56	MG	1A	3651	1/1	0.88	0.09	41,41,41,41	0
56	MG	2A	3364	1/1	0.88	0.11	53,53,53,53	0
56	MG	1A	3005	1/1	0.88	0.33	53,53,53,53	0
56	MG	1A	3117	1/1	0.88	0.16	46,46,46,46	0
56	MG	1A	3431	1/1	0.88	0.15	42,42,42,42	0
56	MG	2A	3293	1/1	0.88	0.19	34,34,34,34	0
56	MG	2A	3514	1/1	0.88	0.13	44,44,44,44	0
56	MG	1A	3176	1/1	0.88	0.16	69,69,69,69	0
56	MG	2A	3450	1/1	0.88	0.14	41,41,41,41	0
56	MG	1A	3444	1/1	0.88	0.35	33,33,33,33	0
56	MG	2A	3601	1/1	0.88	0.23	52,52,52,52	0
56	MG	2A	3248	1/1	0.88	0.11	40,40,40,40	0
56	MG	2A	3059	1/1	0.88	0.14	44,44,44,44	0
56	MG	1a	1682	1/1	0.88	0.19	35,35,35,35	0
56	MG	1A	3335	1/1	0.88	0.14	44,44,44,44	0
56	MG	2A	3160	1/1	0.88	0.45	56,56,56,56	0
56	MG	2A	3436	1/1	0.88	0.34	40,40,40,40	0
56	MG	2A	3070	1/1	0.88	0.24	42,42,42,42	0
56	MG	1A	3704	1/1	0.88	0.14	45,45,45,45	0
56	MG	2A	3235	1/1	0.88	0.36	48,48,48,48	0
56	MG	2F	301	1/1	0.88	0.25	44,44,44,44	0
56	MG	1A	3040	1/1	0.88	0.14	49,49,49,49	0
56	MG	1A	3430	1/1	0.88	0.14	64,64,64,64	0
56	MG	2A	3133	1/1	0.88	0.66	47,47,47,47	0
56	MG	1A	3428	1/1	0.88	0.32	58,58,58,58	0
56	MG	1A	3633	1/1	0.88	0.10	34,34,34,34	0
56	MG	2A	3435	1/1	0.88	0.28	49,49,49,49	0
56	MG	2A	3174	1/1	0.88	0.13	49,49,49,49	0
56	MG	1A	3180	1/1	0.88	0.29	38,38,38,38	0
56	MG	1A	3337	1/1	0.89	0.15	31,31,31,31	0
56	MG	2A	3622	1/1	0.89	0.24	55,55,55,55	0
56	MG	1A	3761	1/1	0.89	0.09	48,48,48,48	0
56	MG	2a	3047	1/1	0.89	0.11	67,67,67,67	0
56	MG	1A	3597	1/1	0.89	0.20	34,34,34,34	0
56	MG	1A	3649	1/1	0.89	0.08	36,36,36,36	0
56	MG	2A	3408	1/1	0.89	0.26	43,43,43,43	0
56	MG	2A	3061	1/1	0.89	0.25	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3329	1/1	0.89	0.16	55,55,55,55	0
56	MG	2a	3073	1/1	0.89	0.11	60,60,60,60	0
56	MG	1a	1683	1/1	0.89	0.17	53,53,53,53	0
56	MG	1A	3759	1/1	0.89	0.07	50,50,50,50	0
56	MG	2B	209	1/1	0.89	0.34	50,50,50,50	0
56	MG	1A	3614	1/1	0.89	0.19	47,47,47,47	0
56	MG	1P	205	1/1	0.89	0.16	36,36,36,36	0
56	MG	1A	3042	1/1	0.89	0.12	33,33,33,33	0
56	MG	2A	3396	1/1	0.89	0.17	52,52,52,52	0
56	MG	2A	3377	1/1	0.89	0.14	47,47,47,47	0
56	MG	27	101	1/1	0.89	0.15	44,44,44,44	0
56	MG	2Z	301	1/1	0.89	0.16	60,60,60,60	0
56	MG	1A	3635	1/1	0.89	0.09	53,53,53,53	0
56	MG	1a	1647	1/1	0.89	0.13	49,49,49,49	0
56	MG	2a	3102	1/1	0.89	0.13	53,53,53,53	0
56	MG	1A	3314	1/1	0.89	0.77	38,38,38,38	0
56	MG	1A	3747	1/1	0.89	0.24	65,65,65,65	0
56	MG	2A	3077	1/1	0.89	0.26	54,54,54,54	0
56	MG	2A	3148	1/1	0.89	0.17	45,45,45,45	0
56	MG	1A	3265	1/1	0.89	0.43	45,45,45,45	0
56	MG	2a	3037	1/1	0.89	0.40	57,57,57,57	0
56	MG	2A	3357	1/1	0.89	0.29	54,54,54,54	0
56	MG	1A	3090	1/1	0.89	0.21	27,27,27,27	0
56	MG	1a	1635	1/1	0.89	0.18	57,57,57,57	0
56	MG	1A	3189	1/1	0.89	0.21	44,44,44,44	0
56	MG	2A	3464	1/1	0.89	0.09	39,39,39,39	0
56	MG	23	102	1/1	0.89	0.50	50,50,50,50	0
56	MG	1A	3339	1/1	0.89	0.14	55,55,55,55	0
56	MG	1A	3355	1/1	0.89	0.96	45,45,45,45	0
56	MG	2A	3114	1/1	0.89	0.10	46,46,46,46	0
56	MG	2a	3131	1/1	0.89	0.29	60,60,60,60	0
56	MG	1a	1637	1/1	0.89	0.08	46,46,46,46	0
56	MG	1A	3052	1/1	0.89	0.14	47,47,47,47	0
56	MG	2A	3573	1/1	0.89	0.11	55,55,55,55	0
56	MG	1A	3793	1/1	0.89	0.11	40,40,40,40	0
56	MG	2A	3158	1/1	0.89	0.14	50,50,50,50	0
56	MG	1A	3032	1/1	0.89	0.18	44,44,44,44	0
56	MG	1A	3336	1/1	0.89	0.31	53,53,53,53	0
56	MG	1Q	202	1/1	0.89	0.21	40,40,40,40	0
56	MG	2A	3343	1/1	0.89	0.23	69,69,69,69	0
56	MG	1A	3142	1/1	0.89	0.18	29,29,29,29	0
56	MG	2A	3090	1/1	0.89	0.23	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1a	1676	1/1	0.89	0.20	46,46,46,46	0
56	MG	2T	201	1/1	0.89	0.15	33,33,33,33	0
56	MG	1n	102	1/1	0.89	0.14	47,47,47,47	0
56	MG	1a	1695	1/1	0.89	0.21	59,59,59,59	0
56	MG	1A	3404	1/1	0.89	0.17	52,52,52,52	0
56	MG	15	102	1/1	0.89	0.50	31,31,31,31	0
56	MG	2A	3469	1/1	0.89	0.15	34,34,34,34	0
56	MG	10	103	1/1	0.89	0.27	58,58,58,58	0
56	MG	1A	3388	1/1	0.89	1.27	35,35,35,35	0
56	MG	1a	1752	1/1	0.89	0.22	60,60,60,60	0
56	MG	1A	3200	1/1	0.89	0.57	46,46,46,46	0
56	MG	1A	3305	1/1	0.89	0.18	32,32,32,32	0
56	MG	2A	3112	1/1	0.89	0.36	51,51,51,51	0
56	MG	1A	3660	1/1	0.89	0.15	63,63,63,63	0
56	MG	1a	1710	1/1	0.89	0.18	55,55,55,55	0
56	MG	2a	3029	1/1	0.89	0.12	47,47,47,47	0
56	MG	2A	3281	1/1	0.89	0.08	38,38,38,38	0
56	MG	1a	1718	1/1	0.89	0.10	53,53,53,53	0
56	MG	2A	3187	1/1	0.89	0.27	56,56,56,56	0
56	MG	2A	3034	1/1	0.89	0.19	34,34,34,34	0
56	MG	1a	1631	1/1	0.89	0.20	56,56,56,56	0
56	MG	1A	3349	1/1	0.89	0.10	46,46,46,46	0
56	MG	2A	3019	1/1	0.89	0.30	51,51,51,51	0
56	MG	1A	3234	1/1	0.89	0.30	44,44,44,44	0
56	MG	1a	1751	1/1	0.89	0.29	60,60,60,60	0
56	MG	1A	3380	1/1	0.90	0.13	53,53,53,53	0
56	MG	2A	3398	1/1	0.90	0.38	52,52,52,52	0
56	MG	1a	1765	1/1	0.90	0.15	62,62,62,62	0
56	MG	1B	203	1/1	0.90	0.14	61,61,61,61	0
56	MG	2a	3087	1/1	0.90	0.14	67,67,67,67	0
56	MG	1A	3081	1/1	0.90	0.20	57,57,57,57	0
56	MG	1a	1735	1/1	0.90	0.13	57,57,57,57	0
56	MG	1A	3615	1/1	0.90	0.14	31,31,31,31	0
56	MG	1A	3479	1/1	0.90	0.08	41,41,41,41	0
56	MG	1a	1755	1/1	0.90	0.20	46,46,46,46	0
56	MG	2a	3049	1/1	0.90	0.17	54,54,54,54	0
56	MG	2A	3324	1/1	0.90	0.14	53,53,53,53	0
56	MG	1A	3076	1/1	0.90	0.17	46,46,46,46	0
56	MG	2E	304	1/1	0.90	0.18	52,52,52,52	0
56	MG	2W	201	1/1	0.90	0.12	45,45,45,45	0
56	MG	1A	3310	1/1	0.90	0.55	46,46,46,46	0
56	MG	2a	3059	1/1	0.90	0.15	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1a	1679	1/1	0.90	0.19	47,47,47,47	0
56	MG	2A	3395	1/1	0.90	0.28	52,52,52,52	0
56	MG	20	101	1/1	0.90	0.17	63,63,63,63	0
56	MG	2a	3015	1/1	0.90	0.07	63,63,63,63	0
56	MG	2A	3564	1/1	0.90	0.09	47,47,47,47	0
56	MG	2a	3035	1/1	0.90	0.23	61,61,61,61	0
56	MG	2A	3009	1/1	0.90	0.18	50,50,50,50	0
56	MG	2A	3153	1/1	0.90	0.15	49,49,49,49	0
56	MG	2A	3006	1/1	0.90	0.26	46,46,46,46	0
56	MG	2A	3139	1/1	0.90	0.17	30,30,30,30	0
56	MG	1A	3692	1/1	0.90	0.51	48,48,48,48	0
56	MG	2A	3401	1/1	0.90	0.26	53,53,53,53	0
56	MG	2A	3023	1/1	0.90	0.13	45,45,45,45	0
56	MG	1A	3717	1/1	0.90	0.21	33,33,33,33	0
56	MG	2A	3454	1/1	0.90	0.11	37,37,37,37	0
56	MG	1V	204	1/1	0.90	0.25	44,44,44,44	0
56	MG	1H	201	1/1	0.90	0.24	40,40,40,40	0
56	MG	2A	3196	1/1	0.90	0.62	53,53,53,53	0
56	MG	1a	1605	1/1	0.90	0.22	54,54,54,54	0
56	MG	2A	3527	1/1	0.90	0.16	44,44,44,44	0
56	MG	2A	3303	1/1	0.90	0.17	48,48,48,48	0
56	MG	2A	3518	1/1	0.90	0.20	55,55,55,55	0
56	MG	1A	3553	1/1	0.90	0.19	65,65,65,65	0
56	MG	1A	3113	1/1	0.90	0.13	58,58,58,58	0
56	MG	1A	3266	1/1	0.90	0.15	47,47,47,47	0
56	MG	1A	3347	1/1	0.90	0.21	62,62,62,62	0
56	MG	1A	3457	1/1	0.90	0.20	45,45,45,45	0
56	MG	1A	3246	1/1	0.90	0.31	34,34,34,34	0
56	MG	1B	214	1/1	0.90	0.24	45,45,45,45	0
56	MG	2A	3101	1/1	0.90	0.11	65,65,65,65	0
56	MG	2a	3092	1/1	0.90	0.18	58,58,58,58	0
56	MG	1A	3174	1/1	0.90	0.41	41,41,41,41	0
56	MG	1a	1640	1/1	0.90	0.14	42,42,42,42	0
56	MG	2E	303	1/1	0.90	0.13	42,42,42,42	0
56	MG	1A	3364	1/1	0.90	0.35	40,40,40,40	0
56	MG	2A	3172	1/1	0.90	0.20	51,51,51,51	0
56	MG	2A	3402	1/1	0.90	0.14	45,45,45,45	0
56	MG	1A	3639	1/1	0.90	0.10	67,67,67,67	0
59	K	2x	101	1/1	0.90	0.59	78,78,78,78	0
56	MG	1A	3437	1/1	0.90	0.35	53,53,53,53	0
56	MG	2A	3121	1/1	0.90	0.11	47,47,47,47	0
56	MG	1A	3460	1/1	0.90	0.19	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3259	1/1	0.90	0.15	60,60,60,60	0
56	MG	1A	3302	1/1	0.90	0.17	55,55,55,55	0
56	MG	1A	3433	1/1	0.90	0.23	41,41,41,41	0
56	MG	1a	1694	1/1	0.90	0.15	35,35,35,35	0
56	MG	1F	311	1/1	0.90	0.60	47,47,47,47	0
56	MG	1F	301	1/1	0.90	0.82	52,52,52,52	0
56	MG	1x	104	1/1	0.90	0.17	58,58,58,58	0
56	MG	2A	3073	1/1	0.90	0.54	43,43,43,43	0
56	MG	1A	3408	1/1	0.90	0.36	65,65,65,65	0
56	MG	2A	3184	1/1	0.90	0.14	67,67,67,67	0
56	MG	1A	3159	1/1	0.90	0.19	37,37,37,37	0
56	MG	1A	3082	1/1	0.90	0.25	44,44,44,44	0
56	MG	2A	3111	1/1	0.90	0.14	38,38,38,38	0
56	MG	1A	3034	1/1	0.90	0.28	41,41,41,41	0
56	MG	2A	3165	1/1	0.90	0.12	44,44,44,44	0
56	MG	1A	3755	1/1	0.90	0.07	55,55,55,55	0
56	MG	1E	307	1/1	0.90	0.15	38,38,38,38	0
56	MG	1A	3706	1/1	0.90	0.20	41,41,41,41	0
56	MG	2a	3076	1/1	0.90	0.25	48,48,48,48	0
56	MG	2A	3419	1/1	0.90	0.18	30,30,30,30	0
56	MG	2A	3142	1/1	0.90	0.11	44,44,44,44	0
56	MG	1A	3765	1/1	0.90	0.15	45,45,45,45	0
56	MG	2A	3314	1/1	0.90	0.31	40,40,40,40	0
56	MG	2A	3232	1/1	0.90	0.16	63,63,63,63	0
56	MG	1a	1756	1/1	0.90	0.32	54,54,54,54	0
56	MG	1A	3037	1/1	0.90	0.16	27,27,27,27	0
56	MG	2D	301	1/1	0.91	0.29	35,35,35,35	0
56	MG	2A	3338	1/1	0.91	0.19	45,45,45,45	0
56	MG	1A	3240	1/1	0.91	0.17	55,55,55,55	0
56	MG	2A	3270	1/1	0.91	0.34	61,61,61,61	0
56	MG	1A	3394	1/1	0.91	0.29	42,42,42,42	0
56	MG	1A	3084	1/1	0.91	0.38	48,48,48,48	0
56	MG	1A	3827	1/1	0.91	0.13	51,51,51,51	0
56	MG	2A	3074	1/1	0.91	0.18	57,57,57,57	0
56	MG	1a	1727	1/1	0.91	0.20	54,54,54,54	0
56	MG	1a	1617	1/1	0.91	0.24	47,47,47,47	0
56	MG	2A	3609	1/1	0.91	0.22	42,42,42,42	0
56	MG	2A	3572	1/1	0.91	0.18	56,56,56,56	0
56	MG	2a	3114	1/1	0.91	0.22	59,59,59,59	0
56	MG	1A	3181	1/1	0.91	0.18	34,34,34,34	0
56	MG	2A	3190	1/1	0.91	0.29	55,55,55,55	0
56	MG	1A	3249	1/1	0.91	0.66	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2a	3125	1/1	0.91	0.25	46,46,46,46	0
56	MG	1V	205	1/1	0.91	0.17	47,47,47,47	0
56	MG	1A	3241	1/1	0.91	0.17	54,54,54,54	0
56	MG	2a	3007	1/1	0.91	0.10	50,50,50,50	0
56	MG	2A	3397	1/1	0.91	0.57	69,69,69,69	0
56	MG	1A	3413	1/1	0.91	0.11	38,38,38,38	0
56	MG	1a	1740	1/1	0.91	0.21	35,35,35,35	0
56	MG	1A	3748	1/1	0.91	0.09	77,77,77,77	0
56	MG	2A	3207	1/1	0.91	0.26	55,55,55,55	0
56	MG	2A	3208	1/1	0.91	0.23	60,60,60,60	0
56	MG	2A	3380	1/1	0.91	0.74	44,44,44,44	0
56	MG	1A	3317	1/1	0.91	0.30	46,46,46,46	0
56	MG	2A	3213	1/1	0.91	0.15	55,55,55,55	0
56	MG	1A	3725	1/1	0.91	0.14	32,32,32,32	0
56	MG	2A	3447	1/1	0.91	0.10	47,47,47,47	0
56	MG	1A	3558	1/1	0.91	0.20	49,49,49,49	0
56	MG	1a	1606	1/1	0.91	0.14	54,54,54,54	0
56	MG	2a	3123	1/1	0.91	0.12	62,62,62,62	0
56	MG	2A	3276	1/1	0.91	0.21	39,39,39,39	0
56	MG	2A	3523	1/1	0.91	0.33	62,62,62,62	0
56	MG	2a	3091	1/1	0.91	0.10	43,43,43,43	0
56	MG	2A	3404	1/1	0.91	0.25	38,38,38,38	0
56	MG	1A	3559	1/1	0.91	0.40	44,44,44,44	0
56	MG	2A	3334	1/1	0.91	0.11	51,51,51,51	0
56	MG	1T	201	1/1	0.91	0.17	44,44,44,44	0
56	MG	2A	3127	1/1	0.91	0.21	44,44,44,44	0
56	MG	1z	101	1/1	0.91	0.24	49,49,49,49	0
56	MG	1A	3806	1/1	0.91	0.11	32,32,32,32	0
56	MG	2A	3537	1/1	0.91	0.26	57,57,57,57	0
56	MG	2A	3069	1/1	0.91	0.22	53,53,53,53	0
56	MG	1A	3389	1/1	0.91	0.22	50,50,50,50	0
56	MG	1A	3533	1/1	0.91	0.12	27,27,27,27	0
56	MG	2A	3585	1/1	0.91	0.12	66,66,66,66	0
56	MG	2A	3024	1/1	0.91	0.18	49,49,49,49	0
56	MG	1a	1660	1/1	0.91	0.44	48,48,48,48	0
56	MG	2Y	201	1/1	0.91	0.27	41,41,41,41	0
56	MG	2F	303	1/1	0.91	0.22	56,56,56,56	0
56	MG	1x	107	1/1	0.91	0.20	48,48,48,48	0
56	MG	10	101	1/1	0.91	0.24	41,41,41,41	0
56	MG	1a	1697	1/1	0.91	0.33	72,72,72,72	0
56	MG	17	3103	1/1	0.91	0.50	37,37,37,37	0
56	MG	2a	3097	1/1	0.91	0.12	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3302	1/1	0.91	0.22	42,42,42,42	0
56	MG	2A	3104	1/1	0.91	0.49	38,38,38,38	0
56	MG	2A	3095	1/1	0.91	0.20	38,38,38,38	0
56	MG	1A	3229	1/1	0.91	0.49	46,46,46,46	0
56	MG	2A	3175	1/1	0.91	0.18	44,44,44,44	0
56	MG	1A	3528	1/1	0.91	0.11	28,28,28,28	0
56	MG	1A	3655	1/1	0.91	0.32	45,45,45,45	0
56	MG	2A	3078	1/1	0.91	0.10	54,54,54,54	0
56	MG	28	103	1/1	0.91	0.15	60,60,60,60	0
56	MG	2A	3465	1/1	0.91	0.09	37,37,37,37	0
56	MG	1A	3094	1/1	0.91	0.56	42,42,42,42	0
56	MG	2A	3131	1/1	0.91	0.18	53,53,53,53	0
56	MG	1A	3279	1/1	0.91	0.29	33,33,33,33	0
56	MG	2A	3382	1/1	0.91	0.16	53,53,53,53	0
56	MG	1A	3530	1/1	0.91	0.16	34,34,34,34	0
56	MG	2A	3378	1/1	0.91	0.23	57,57,57,57	0
56	MG	1A	3808	1/1	0.91	0.14	45,45,45,45	0
56	MG	1A	3669	1/1	0.91	0.46	38,38,38,38	0
56	MG	1A	3512	1/1	0.91	0.09	50,50,50,50	0
56	MG	2a	3098	1/1	0.91	0.12	45,45,45,45	0
56	MG	2A	3403	1/1	0.91	0.12	48,48,48,48	0
56	MG	28	101	1/1	0.91	0.16	50,50,50,50	0
56	MG	17	3101	1/1	0.91	0.18	33,33,33,33	0
56	MG	2l	202	1/1	0.91	0.15	44,44,44,44	0
56	MG	1Q	204	1/1	0.91	0.39	41,41,41,41	0
56	MG	1A	3290	1/1	0.91	0.21	45,45,45,45	0
56	MG	2A	3385	1/1	0.91	0.15	53,53,53,53	0
56	MG	1a	1626	1/1	0.91	0.12	35,35,35,35	0
56	MG	1A	3712	1/1	0.91	0.72	43,43,43,43	0
56	MG	1A	3709	1/1	0.91	0.22	41,41,41,41	0
56	MG	1A	3182	1/1	0.91	0.13	47,47,47,47	0
56	MG	1a	1753	1/1	0.91	0.20	59,59,59,59	0
56	MG	1A	3318	1/1	0.91	0.15	38,38,38,38	0
56	MG	1A	3360	1/1	0.91	0.19	29,29,29,29	0
56	MG	1A	3269	1/1	0.91	0.20	34,34,34,34	0
56	MG	1h	201	1/1	0.91	0.12	54,54,54,54	0
56	MG	1a	1658	1/1	0.91	0.27	59,59,59,59	0
56	MG	18	103	1/1	0.91	0.13	62,62,62,62	0
56	MG	1A	3287	1/1	0.91	0.72	44,44,44,44	0
56	MG	1A	3801	1/1	0.91	0.10	47,47,47,47	0
56	MG	2A	3277	1/1	0.91	0.23	37,37,37,37	0
56	MG	2A	3587	1/1	0.91	0.13	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3488	1/1	0.91	0.11	36,36,36,36	0
56	MG	1a	1757	1/1	0.91	0.23	51,51,51,51	0
56	MG	2A	3406	1/1	0.91	0.29	50,50,50,50	0
56	MG	2A	3332	1/1	0.91	0.12	56,56,56,56	0
56	MG	2A	3005	1/1	0.91	0.20	42,42,42,42	0
56	MG	1A	3745	1/1	0.91	0.14	51,51,51,51	0
56	MG	1N	201	1/1	0.91	0.61	45,45,45,45	0
56	MG	1a	1650	1/1	0.91	0.11	45,45,45,45	0
56	MG	1l	202	1/1	0.91	0.12	53,53,53,53	0
56	MG	1a	1730	1/1	0.91	0.09	67,67,67,67	0
56	MG	1a	1667	1/1	0.91	0.20	49,49,49,49	0
56	MG	1A	3049	1/1	0.91	0.21	47,47,47,47	0
56	MG	2A	3113	1/1	0.91	0.35	68,68,68,68	0
56	MG	2A	3224	1/1	0.91	0.12	48,48,48,48	0
56	MG	2A	3614	1/1	0.92	0.16	38,38,38,38	0
56	MG	2a	3138	1/1	0.92	0.15	67,67,67,67	0
56	MG	2a	3016	1/1	0.92	0.11	76,76,76,76	0
56	MG	2A	3243	1/1	0.92	0.12	54,54,54,54	0
56	MG	2f	201	1/1	0.92	0.07	54,54,54,54	0
56	MG	13	103	1/1	0.92	0.12	38,38,38,38	0
56	MG	1a	1655	1/1	0.92	0.22	56,56,56,56	0
56	MG	1A	3777	1/1	0.92	0.20	45,45,45,45	0
56	MG	1a	1696	1/1	0.92	0.13	51,51,51,51	0
56	MG	1A	3050	1/1	0.92	0.16	49,49,49,49	0
56	MG	2a	3034	1/1	0.92	0.14	57,57,57,57	0
56	MG	1A	3334	1/1	0.92	0.11	34,34,34,34	0
56	MG	2A	3230	1/1	0.92	0.18	46,46,46,46	0
56	MG	2A	3161	1/1	0.92	0.24	48,48,48,48	0
56	MG	2A	3610	1/1	0.92	0.12	46,46,46,46	0
56	MG	1A	3033	1/1	0.92	0.12	43,43,43,43	0
56	MG	2a	3103	1/1	0.92	0.12	65,65,65,65	0
56	MG	1A	3170	1/1	0.92	0.63	33,33,33,33	0
56	MG	2A	3389	1/1	0.92	0.14	45,45,45,45	0
56	MG	1A	3298	1/1	0.92	0.27	55,55,55,55	0
56	MG	1A	3749	1/1	0.92	0.09	78,78,78,78	0
56	MG	2a	3100	1/1	0.92	0.09	35,35,35,35	0
56	MG	2A	3100	1/1	0.92	0.20	34,34,34,34	0
56	MG	1A	3315	1/1	0.92	0.34	46,46,46,46	0
56	MG	1A	3613	1/1	0.92	0.13	27,27,27,27	0
56	MG	1A	3321	1/1	0.92	0.51	43,43,43,43	0
56	MG	1A	3214	1/1	0.92	0.11	46,46,46,46	0
56	MG	1A	3593	1/1	0.92	0.12	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3393	1/1	0.92	0.28	30,30,30,30	0
56	MG	1A	3500	1/1	0.92	0.12	59,59,59,59	0
56	MG	2a	3085	1/1	0.92	0.19	52,52,52,52	0
56	MG	2a	3011	1/1	0.92	0.11	62,62,62,62	0
56	MG	1a	1705	1/1	0.92	0.21	52,52,52,52	0
56	MG	1A	3112	1/1	0.92	0.51	36,36,36,36	0
56	MG	1A	3154	1/1	0.92	0.28	42,42,42,42	0
56	MG	1A	3605	1/1	0.92	0.16	29,29,29,29	0
56	MG	1G	201	1/1	0.92	0.17	32,32,32,32	0
56	MG	1A	3825	1/1	0.92	0.21	46,46,46,46	0
56	MG	1A	3102	1/1	0.92	0.09	42,42,42,42	0
56	MG	2A	3589	1/1	0.92	0.08	32,32,32,32	0
56	MG	2A	3241	1/1	0.92	0.28	42,42,42,42	0
56	MG	1A	3224	1/1	0.92	0.14	33,33,33,33	0
56	MG	2A	3135	1/1	0.92	0.24	52,52,52,52	0
56	MG	1A	3365	1/1	0.92	0.14	30,30,30,30	0
56	MG	1A	3529	1/1	0.92	0.14	20,20,20,20	0
56	MG	2A	3278	1/1	0.92	0.23	23,23,23,23	0
56	MG	1A	3158	1/1	0.92	1.01	36,36,36,36	0
56	MG	1A	3361	1/1	0.92	0.08	46,46,46,46	0
56	MG	1a	1741	1/1	0.92	0.19	46,46,46,46	0
56	MG	1A	3516	1/1	0.92	0.14	25,25,25,25	0
56	MG	2A	3373	1/1	0.92	0.14	34,34,34,34	0
56	MG	2A	3489	1/1	0.92	0.12	54,54,54,54	0
56	MG	2B	210	1/1	0.92	0.13	58,58,58,58	0
56	MG	1A	3333	1/1	0.92	0.68	37,37,37,37	0
56	MG	2A	3168	1/1	0.92	0.11	54,54,54,54	0
56	MG	1A	3576	1/1	0.92	0.12	46,46,46,46	0
56	MG	1A	3296	1/1	0.92	0.14	61,61,61,61	0
56	MG	1A	3582	1/1	0.92	0.07	72,72,72,72	0
56	MG	1B	220	1/1	0.92	0.15	53,53,53,53	0
56	MG	1A	3819	1/1	0.92	0.19	61,61,61,61	0
56	MG	2A	3128	1/1	0.92	0.27	47,47,47,47	0
56	MG	1A	3350	1/1	0.92	0.19	36,36,36,36	0
56	MG	1A	3799	1/1	0.92	0.11	49,49,49,49	0
56	MG	1B	210	1/1	0.92	0.14	41,41,41,41	0
56	MG	2A	3102	1/1	0.92	0.21	50,50,50,50	0
56	MG	1A	3410	1/1	0.92	0.20	45,45,45,45	0
56	MG	1A	3626	1/1	0.92	0.18	28,28,28,28	0
56	MG	1a	1702	1/1	0.92	0.18	42,42,42,42	0
56	MG	1A	3724	1/1	0.92	0.09	26,26,26,26	0
56	MG	1a	1673	1/1	0.92	0.19	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3691	1/1	0.92	0.15	46,46,46,46	0
56	MG	2a	3002	1/1	0.92	0.10	55,55,55,55	0
56	MG	1D	306	1/1	0.92	0.80	47,47,47,47	0
56	MG	2A	3171	1/1	0.92	0.34	45,45,45,45	0
56	MG	1A	3327	1/1	0.92	0.65	41,41,41,41	0
56	MG	2a	3031	1/1	0.92	0.11	46,46,46,46	0
56	MG	2A	3577	1/1	0.92	0.13	65,65,65,65	0
56	MG	1A	3053	1/1	0.92	0.11	32,32,32,32	0
56	MG	2A	3504	1/1	0.92	0.14	43,43,43,43	0
56	MG	2A	3189	1/1	0.92	0.27	49,49,49,49	0
56	MG	2A	3003	1/1	0.92	0.14	45,45,45,45	0
56	MG	1A	3213	1/1	0.92	0.10	33,33,33,33	0
56	MG	1A	3316	1/1	0.92	0.25	45,45,45,45	0
56	MG	2B	208	1/1	0.92	0.15	68,68,68,68	0
56	MG	2A	3374	1/1	0.92	0.10	47,47,47,47	0
56	MG	2a	3010	1/1	0.92	0.13	44,44,44,44	0
56	MG	1B	223	1/1	0.92	0.14	34,34,34,34	0
56	MG	1a	1734	1/1	0.92	0.19	45,45,45,45	0
56	MG	1A	3435	1/1	0.92	0.36	45,45,45,45	0
56	MG	2A	3212	1/1	0.92	0.12	62,62,62,62	0
56	MG	1A	3253	1/1	0.92	0.47	44,44,44,44	0
56	MG	2A	3350	1/1	0.92	0.08	42,42,42,42	0
56	MG	1A	3077	1/1	0.92	0.10	36,36,36,36	0
56	MG	2A	3200	1/1	0.92	0.09	46,46,46,46	0
56	MG	2A	3183	1/1	0.92	0.12	50,50,50,50	0
56	MG	2A	3109	1/1	0.92	0.30	53,53,53,53	0
56	MG	2A	3156	1/1	0.92	0.11	48,48,48,48	0
56	MG	1A	3821	1/1	0.92	0.12	54,54,54,54	0
56	MG	2x	103	1/1	0.92	0.16	51,51,51,51	0
56	MG	2a	3118	1/1	0.92	0.19	61,61,61,61	0
56	MG	2A	3054	1/1	0.92	0.21	51,51,51,51	0
56	MG	2A	3105	1/1	0.92	0.27	37,37,37,37	0
56	MG	1W	202	1/1	0.92	0.55	40,40,40,40	0
56	MG	2a	3017	1/1	0.92	0.17	50,50,50,50	0
56	MG	2a	3071	1/1	0.92	0.15	44,44,44,44	0
56	MG	2A	3144	1/1	0.92	0.28	35,35,35,35	0
56	MG	2A	3031	1/1	0.92	0.08	44,44,44,44	0
56	MG	1A	3055	1/1	0.92	0.13	48,48,48,48	0
56	MG	1A	3128	1/1	0.92	0.19	51,51,51,51	0
56	MG	1A	3054	1/1	0.92	0.12	55,55,55,55	0
56	MG	1A	3089	1/1	0.92	0.91	51,51,51,51	0
56	MG	1A	3604	1/1	0.92	0.15	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3673	1/1	0.92	0.17	64,64,64,64	0
56	MG	1B	211	1/1	0.92	0.31	39,39,39,39	0
56	MG	2A	3260	1/1	0.92	0.47	53,53,53,53	0
56	MG	1A	3222	1/1	0.92	0.12	40,40,40,40	0
56	MG	1A	3236	1/1	0.92	0.21	45,45,45,45	0
56	MG	1a	1758	1/1	0.92	0.39	49,49,49,49	0
56	MG	1a	1649	1/1	0.92	0.20	51,51,51,51	0
56	MG	2a	3063	1/1	0.92	0.20	64,64,64,64	0
56	MG	2A	3432	1/1	0.92	0.21	30,30,30,30	0
56	MG	1A	3134	1/1	0.92	0.46	32,32,32,32	0
56	MG	1A	3440	1/1	0.92	0.14	46,46,46,46	0
56	MG	1E	304	1/1	0.92	0.18	42,42,42,42	0
56	MG	1A	3807	1/1	0.92	0.17	24,24,24,24	0
56	MG	1a	1653	1/1	0.92	0.11	42,42,42,42	0
56	MG	1A	3716	1/1	0.92	0.16	53,53,53,53	0
56	MG	1A	3738	1/1	0.92	0.33	44,44,44,44	0
56	MG	1A	3731	1/1	0.92	0.08	65,65,65,65	0
56	MG	1F	302	1/1	0.92	0.42	45,45,45,45	0
56	MG	2I	201	1/1	0.92	0.32	43,43,43,43	0
56	MG	1A	3002	1/1	0.92	0.27	56,56,56,56	0
56	MG	1A	3625	1/1	0.92	0.11	24,24,24,24	0
56	MG	1A	3325	1/1	0.92	0.14	52,52,52,52	0
56	MG	2A	3040	1/1	0.92	0.22	55,55,55,55	0
56	MG	1A	3640	1/1	0.92	0.14	30,30,30,30	0
56	MG	1A	3199	1/1	0.92	0.26	74,74,74,74	0
56	MG	1U	202	1/1	0.92	0.35	32,32,32,32	0
56	MG	1A	3343	1/1	0.92	0.17	34,34,34,34	0
56	MG	1A	3354	1/1	0.92	0.34	40,40,40,40	0
56	MG	1A	3028	1/1	0.92	0.10	44,44,44,44	0
56	MG	1a	1607	1/1	0.92	0.19	47,47,47,47	0
56	MG	1R	203	1/1	0.92	0.24	50,50,50,50	0
56	MG	2A	3431	1/1	0.92	0.12	44,44,44,44	0
56	MG	1A	3295	1/1	0.92	0.18	45,45,45,45	0
56	MG	2B	207	1/1	0.92	0.12	57,57,57,57	0
56	MG	2A	3201	1/1	0.92	0.18	46,46,46,46	0
56	MG	1A	3752	1/1	0.92	0.23	73,73,73,73	0
56	MG	1a	1666	1/1	0.93	0.27	31,31,31,31	0
56	MG	2A	3042	1/1	0.93	0.12	31,31,31,31	0
56	MG	2A	3234	1/1	0.93	0.11	41,41,41,41	0
56	MG	2a	3128	1/1	0.93	0.20	47,47,47,47	0
56	MG	2A	3267	1/1	0.93	0.34	51,51,51,51	0
56	MG	1A	3311	1/1	0.93	0.31	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1f	201	1/1	0.93	0.10	61,61,61,61	0
56	MG	2A	3211	1/1	0.93	0.10	51,51,51,51	0
56	MG	2A	3266	1/1	0.93	0.17	38,38,38,38	0
56	MG	1W	204	1/1	0.93	0.29	53,53,53,53	0
56	MG	2A	3313	1/1	0.93	0.10	51,51,51,51	0
56	MG	1A	3662	1/1	0.93	0.09	61,61,61,61	0
56	MG	2A	3578	1/1	0.93	0.13	60,60,60,60	0
56	MG	2A	3192	1/1	0.93	0.09	43,43,43,43	0
56	MG	1I	201	1/1	0.93	0.07	55,55,55,55	0
56	MG	2A	3615	1/1	0.93	0.19	59,59,59,59	0
56	MG	2a	3060	1/1	0.93	0.14	49,49,49,49	0
56	MG	1A	3193	1/1	0.93	0.18	34,34,34,34	0
56	MG	1A	3598	1/1	0.93	0.13	40,40,40,40	0
56	MG	1A	3734	1/1	0.93	0.10	45,45,45,45	0
56	MG	2a	3104	1/1	0.93	0.26	45,45,45,45	0
56	MG	1V	203	1/1	0.93	0.15	41,41,41,41	0
56	MG	2A	3434	1/1	0.93	0.13	45,45,45,45	0
56	MG	2a	3145	1/1	0.93	0.19	66,66,66,66	0
56	MG	1A	3203	1/1	0.93	0.28	41,41,41,41	0
56	MG	1A	3568	1/1	0.93	0.23	47,47,47,47	0
56	MG	1a	1608	1/1	0.93	0.10	50,50,50,50	0
56	MG	1A	3545	1/1	0.93	0.23	48,48,48,48	0
56	MG	1A	3587	1/1	0.93	0.08	44,44,44,44	0
56	MG	1A	3175	1/1	0.93	0.18	58,58,58,58	0
56	MG	2A	3002	1/1	0.93	0.24	47,47,47,47	0
56	MG	1A	3654	1/1	0.93	0.10	42,42,42,42	0
56	MG	2A	3565	1/1	0.93	0.15	44,44,44,44	0
56	MG	2A	3455	1/1	0.93	0.11	39,39,39,39	0
56	MG	1A	3156	1/1	0.93	0.12	51,51,51,51	0
56	MG	2A	3411	1/1	0.93	0.15	46,46,46,46	0
56	MG	2A	3386	1/1	0.93	0.11	63,63,63,63	0
56	MG	2A	3179	1/1	0.93	0.17	54,54,54,54	0
56	MG	1R	204	1/1	0.93	0.17	51,51,51,51	0
56	MG	1F	308	1/1	0.93	0.20	33,33,33,33	0
56	MG	2A	3541	1/1	0.93	0.14	38,38,38,38	0
56	MG	1A	3514	1/1	0.93	0.13	25,25,25,25	0
56	MG	2A	3021	1/1	0.93	0.17	53,53,53,53	0
56	MG	1B	221	1/1	0.93	0.08	63,63,63,63	0
56	MG	2A	3296	1/1	0.93	0.21	44,44,44,44	0
56	MG	1A	3312	1/1	0.93	0.12	51,51,51,51	0
56	MG	1A	3161	1/1	0.93	0.12	36,36,36,36	0
56	MG	2A	3272	1/1	0.93	0.21	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2a	3113	1/1	0.93	0.11	59,59,59,59	0
56	MG	2A	3538	1/1	0.93	0.14	44,44,44,44	0
56	MG	2A	3236	1/1	0.93	0.22	46,46,46,46	0
56	MG	1A	3589	1/1	0.93	0.14	67,67,67,67	0
56	MG	2A	3249	1/1	0.93	0.14	49,49,49,49	0
56	MG	1A	3155	1/1	0.93	0.30	47,47,47,47	0
56	MG	2A	3089	1/1	0.93	0.70	51,51,51,51	0
56	MG	1A	3183	1/1	0.93	0.32	55,55,55,55	0
56	MG	1P	201	1/1	0.93	0.66	36,36,36,36	0
56	MG	2A	3606	1/1	0.93	0.25	54,54,54,54	0
56	MG	2A	3244	1/1	0.93	0.26	46,46,46,46	0
56	MG	1A	3143	1/1	0.93	0.13	41,41,41,41	0
56	MG	1A	3452	1/1	0.93	0.20	44,44,44,44	0
56	MG	2A	3129	1/1	0.93	0.26	42,42,42,42	0
56	MG	1a	1688	1/1	0.93	0.14	61,61,61,61	0
56	MG	2a	3027	1/1	0.93	0.14	47,47,47,47	0
56	MG	1A	3013	1/1	0.93	0.72	34,34,34,34	0
56	MG	1A	3085	1/1	0.93	0.73	34,34,34,34	0
56	MG	1A	3027	1/1	0.93	0.20	30,30,30,30	0
56	MG	1A	3844	1/1	0.93	0.16	50,50,50,50	0
56	MG	2A	3030	1/1	0.93	0.10	54,54,54,54	0
56	MG	2A	3166	1/1	0.93	0.24	72,72,72,72	0
56	MG	1N	202	1/1	0.93	0.43	41,41,41,41	0
57	ZN	2n	501	1/1	0.93	0.12	96,96,96,96	0
56	MG	2A	3311	1/1	0.93	0.15	54,54,54,54	0
56	MG	2A	3478	1/1	0.93	0.09	56,56,56,56	0
56	MG	2A	3569	1/1	0.93	0.08	41,41,41,41	0
56	MG	2A	3237	1/1	0.93	0.30	57,57,57,57	0
56	MG	2a	3030	1/1	0.93	0.13	56,56,56,56	0
56	MG	1E	302	1/1	0.93	0.44	34,34,34,34	0
56	MG	1a	1618	1/1	0.93	0.14	61,61,61,61	0
56	MG	1A	3280	1/1	0.93	0.27	34,34,34,34	0
56	MG	2A	3607	1/1	0.93	0.19	49,49,49,49	0
56	MG	2a	3074	1/1	0.93	0.18	40,40,40,40	0
56	MG	1A	3829	1/1	0.93	0.10	54,54,54,54	0
56	MG	2A	3143	1/1	0.93	0.19	56,56,56,56	0
56	MG	1A	3781	1/1	0.93	0.11	39,39,39,39	0
56	MG	2A	3080	1/1	0.93	0.16	44,44,44,44	0
56	MG	1A	3198	1/1	0.93	0.09	41,41,41,41	0
56	MG	1x	108	1/1	0.93	0.32	44,44,44,44	0
56	MG	2D	302	1/1	0.93	0.12	32,32,32,32	0
56	MG	2A	3055	1/1	0.93	0.83	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3228	1/1	0.93	0.15	59,59,59,59	0
56	MG	1A	3661	1/1	0.93	0.31	47,47,47,47	0
56	MG	1a	1713	1/1	0.93	0.15	50,50,50,50	0
56	MG	1A	3103	1/1	0.93	0.10	25,25,25,25	0
56	MG	2B	205	1/1	0.93	0.13	79,79,79,79	0
56	MG	2a	3052	1/1	0.93	0.11	56,56,56,56	0
56	MG	2a	3065	1/1	0.93	0.16	56,56,56,56	0
56	MG	13	102	1/1	0.93	0.15	40,40,40,40	0
56	MG	2a	3142	1/1	0.93	0.22	49,49,49,49	0
56	MG	2A	3036	1/1	0.93	0.17	55,55,55,55	0
56	MG	2A	3275	1/1	0.93	0.60	56,56,56,56	0
56	MG	2a	3111	1/1	0.93	0.12	66,66,66,66	0
56	MG	2A	3305	1/1	0.93	0.32	43,43,43,43	0
56	MG	1B	208	1/1	0.93	0.07	55,55,55,55	0
56	MG	1A	3137	1/1	0.93	0.30	33,33,33,33	0
56	MG	1A	3219	1/1	0.93	0.37	48,48,48,48	0
56	MG	1A	3423	1/1	0.93	0.24	24,24,24,24	0
56	MG	2A	3328	1/1	0.93	0.21	57,57,57,57	0
56	MG	2a	3134	1/1	0.93	0.20	58,58,58,58	0
56	MG	1A	3319	1/1	0.93	0.13	52,52,52,52	0
56	MG	1A	3434	1/1	0.93	0.16	53,53,53,53	0
56	MG	1a	1625	1/1	0.93	0.16	52,52,52,52	0
56	MG	1A	3467	1/1	0.93	0.15	30,30,30,30	0
56	MG	2a	3136	1/1	0.93	0.11	62,62,62,62	0
56	MG	1A	3309	1/1	0.93	0.12	50,50,50,50	0
56	MG	2B	204	1/1	0.93	0.10	62,62,62,62	0
56	MG	1A	3622	1/1	0.93	0.13	39,39,39,39	0
56	MG	1A	3275	1/1	0.93	0.45	55,55,55,55	0
56	MG	1A	3344	1/1	0.93	0.14	32,32,32,32	0
56	MG	1A	3720	1/1	0.93	0.24	49,49,49,49	0
56	MG	2A	3599	1/1	0.93	0.11	45,45,45,45	0
56	MG	1A	3209	1/1	0.93	0.21	40,40,40,40	0
56	MG	1A	3400	1/1	0.93	0.21	54,54,54,54	0
56	MG	2A	3304	1/1	0.93	0.34	49,49,49,49	0
56	MG	2A	3570	1/1	0.93	0.71	79,79,79,79	0
56	MG	1A	3083	1/1	0.93	0.18	52,52,52,52	0
56	MG	2A	3574	1/1	0.93	0.24	60,60,60,60	0
56	MG	2A	3336	1/1	0.93	0.16	64,64,64,64	0
56	MG	1A	3332	1/1	0.93	0.33	50,50,50,50	0
56	MG	1A	3549	1/1	0.93	0.23	54,54,54,54	0
56	MG	2A	3414	1/1	0.93	0.10	45,45,45,45	0
56	MG	1A	3621	1/1	0.93	0.08	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1l	203	1/1	0.93	0.19	41,41,41,41	0
56	MG	1A	3816	1/1	0.93	0.10	55,55,55,55	0
56	MG	1A	3453	1/1	0.93	0.25	48,48,48,48	0
56	MG	1A	3696	1/1	0.93	0.15	67,67,67,67	0
56	MG	2A	3604	1/1	0.93	0.11	51,51,51,51	0
56	MG	1B	219	1/1	0.93	0.18	66,66,66,66	0
56	MG	1A	3464	1/1	0.93	0.18	59,59,59,59	0
56	MG	15	103	1/1	0.93	0.68	41,41,41,41	0
56	MG	1A	3148	1/1	0.93	0.16	38,38,38,38	0
56	MG	2A	3365	1/1	0.93	0.07	69,69,69,69	0
56	MG	1a	1763	1/1	0.93	0.13	59,59,59,59	0
56	MG	1A	3822	1/1	0.93	0.14	40,40,40,40	0
56	MG	1A	3756	1/1	0.94	0.15	29,29,29,29	0
56	MG	1A	3184	1/1	0.94	0.54	46,46,46,46	0
56	MG	2a	3014	1/1	0.94	0.16	35,35,35,35	0
56	MG	1a	1648	1/1	0.94	0.08	52,52,52,52	0
56	MG	2A	3170	1/1	0.94	0.16	46,46,46,46	0
56	MG	2A	3543	1/1	0.94	0.23	58,58,58,58	0
56	MG	2A	3485	1/1	0.94	0.09	58,58,58,58	0
56	MG	2A	3106	1/1	0.94	0.14	33,33,33,33	0
56	MG	1A	3527	1/1	0.94	0.16	23,23,23,23	0
56	MG	1a	1603	1/1	0.94	0.13	59,59,59,59	0
56	MG	1B	224	1/1	0.94	0.14	42,42,42,42	0
56	MG	1A	3541	1/1	0.94	0.15	30,30,30,30	0
56	MG	1A	3843	1/1	0.94	0.12	43,43,43,43	0
56	MG	1A	3466	1/1	0.94	0.20	45,45,45,45	0
56	MG	2A	3020	1/1	0.94	0.11	40,40,40,40	0
56	MG	1A	3803	1/1	0.94	0.22	39,39,39,39	0
56	MG	1V	202	1/1	0.94	0.66	34,34,34,34	0
56	MG	1A	3770	1/1	0.94	0.09	65,65,65,65	0
56	MG	1A	3830	1/1	0.94	0.09	52,52,52,52	0
56	MG	1A	3276	1/1	0.94	0.10	45,45,45,45	0
56	MG	2A	3014	1/1	0.94	0.17	56,56,56,56	0
56	MG	1a	1692	1/1	0.94	0.20	43,43,43,43	0
56	MG	2a	3056	1/1	0.94	0.22	59,59,59,59	0
56	MG	2a	3108	1/1	0.94	0.18	48,48,48,48	0
56	MG	1V	201	1/1	0.94	0.35	38,38,38,38	0
56	MG	1A	3169	1/1	0.94	0.12	50,50,50,50	0
56	MG	2A	3119	1/1	0.94	0.12	42,42,42,42	0
56	MG	1A	3623	1/1	0.94	0.08	65,65,65,65	0
56	MG	1A	3469	1/1	0.94	0.20	48,48,48,48	0
56	MG	1a	1732	1/1	0.94	0.18	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3028	1/1	0.94	0.22	57,57,57,57	0
56	MG	2a	3083	1/1	0.94	0.28	40,40,40,40	0
56	MG	1a	1659	1/1	0.94	0.14	64,64,64,64	0
56	MG	2A	3138	1/1	0.94	0.19	32,32,32,32	0
56	MG	1A	3252	1/1	0.94	0.19	58,58,58,58	0
56	MG	1A	3778	1/1	0.94	0.09	35,35,35,35	0
56	MG	1A	3421	1/1	0.94	0.15	21,21,21,21	0
56	MG	1A	3760	1/1	0.94	0.18	50,50,50,50	0
56	MG	1a	1657	1/1	0.94	0.11	58,58,58,58	0
56	MG	2A	3052	1/1	0.94	0.17	32,32,32,32	0
56	MG	1A	3740	1/1	0.94	0.64	49,49,49,49	0
56	MG	1A	3078	1/1	0.94	0.16	43,43,43,43	0
56	MG	1A	3106	1/1	0.94	0.59	35,35,35,35	0
56	MG	2A	3462	1/1	0.94	0.10	60,60,60,60	0
56	MG	1A	3776	1/1	0.94	0.12	34,34,34,34	0
56	MG	1A	3015	1/1	0.94	0.14	40,40,40,40	0
56	MG	1A	3794	1/1	0.94	0.10	45,45,45,45	0
56	MG	2A	3491	1/1	0.94	0.26	36,36,36,36	0
56	MG	1A	3366	1/1	0.94	0.16	46,46,46,46	0
56	MG	1A	3764	1/1	0.94	0.11	62,62,62,62	0
56	MG	1A	3693	1/1	0.94	0.16	23,23,23,23	0
56	MG	1Q	201	1/1	0.94	0.20	34,34,34,34	0
56	MG	2A	3044	1/1	0.94	0.15	50,50,50,50	0
56	MG	2A	3118	1/1	0.94	0.08	42,42,42,42	0
56	MG	1l	101	1/1	0.94	0.20	36,36,36,36	0
56	MG	2A	3495	1/1	0.94	0.12	44,44,44,44	0
56	MG	2A	3226	1/1	0.94	0.18	27,27,27,27	0
56	MG	1A	3565	1/1	0.94	0.09	45,45,45,45	0
56	MG	1a	1749	1/1	0.94	0.23	31,31,31,31	0
56	MG	2a	3144	1/1	0.94	0.10	45,45,45,45	0
56	MG	2A	3522	1/1	0.94	0.27	41,41,41,41	0
56	MG	2A	3561	1/1	0.94	0.14	51,51,51,51	0
56	MG	2T	202	1/1	0.94	0.22	50,50,50,50	0
56	MG	2A	3141	1/1	0.94	0.26	39,39,39,39	0
56	MG	2A	3289	1/1	0.94	0.11	45,45,45,45	0
56	MG	1a	1604	1/1	0.94	0.14	49,49,49,49	0
56	MG	1A	3657	1/1	0.94	0.18	45,45,45,45	0
56	MG	1A	3221	1/1	0.94	0.46	36,36,36,36	0
56	MG	2A	3392	1/1	0.94	0.44	31,31,31,31	0
56	MG	2A	3384	1/1	0.94	0.24	45,45,45,45	0
56	MG	1A	3792	1/1	0.94	0.14	25,25,25,25	0
56	MG	2A	3367	1/1	0.94	0.43	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3530	1/1	0.94	0.13	39,39,39,39	0
56	MG	1A	3570	1/1	0.94	0.09	48,48,48,48	0
56	MG	2a	3117	1/1	0.94	0.23	50,50,50,50	0
56	MG	2A	3560	1/1	0.94	0.11	75,75,75,75	0
56	MG	2A	3548	1/1	0.94	0.15	67,67,67,67	0
56	MG	1A	3110	1/1	0.94	0.08	42,42,42,42	0
56	MG	1A	3624	1/1	0.94	0.46	60,60,60,60	0
56	MG	17	3106	1/1	0.94	0.60	58,58,58,58	0
56	MG	1A	3680	1/1	0.94	0.14	38,38,38,38	0
56	MG	2a	3050	1/1	0.94	0.26	31,31,31,31	0
56	MG	2A	3125	1/1	0.94	0.20	49,49,49,49	0
56	MG	1A	3449	1/1	0.94	0.14	45,45,45,45	0
56	MG	2A	3429	1/1	0.94	0.27	59,59,59,59	0
56	MG	1A	3493	1/1	0.94	0.17	30,30,30,30	0
56	MG	1A	3291	1/1	0.94	0.61	33,33,33,33	0
56	MG	2A	3459	1/1	0.94	0.13	46,46,46,46	0
56	MG	1O	201	1/1	0.94	0.14	43,43,43,43	0
56	MG	1A	3702	1/1	0.94	0.08	31,31,31,31	0
56	MG	10	102	1/1	0.94	0.38	49,49,49,49	0
56	MG	2A	3519	1/1	0.94	0.12	29,29,29,29	0
56	MG	1A	3526	1/1	0.94	0.13	16,16,16,16	0
56	MG	2a	3032	1/1	0.94	0.21	56,56,56,56	0
56	MG	1A	3201	1/1	0.94	0.51	40,40,40,40	0
56	MG	1A	3448	1/1	0.94	0.14	17,17,17,17	0
56	MG	2a	3115	1/1	0.94	0.10	58,58,58,58	0
56	MG	1A	3658	1/1	0.94	0.13	48,48,48,48	0
56	MG	2a	3061	1/1	0.94	0.24	51,51,51,51	0
56	MG	1A	3043	1/1	0.94	0.11	45,45,45,45	0
56	MG	1A	3218	1/1	0.94	0.12	39,39,39,39	0
56	MG	2A	3412	1/1	0.94	0.09	34,34,34,34	0
56	MG	1A	3436	1/1	0.94	0.23	36,36,36,36	0
56	MG	1A	3168	1/1	0.94	0.07	50,50,50,50	0
56	MG	2A	3540	1/1	0.94	0.17	39,39,39,39	0
56	MG	2A	3094	1/1	0.94	0.15	45,45,45,45	0
56	MG	1A	3036	1/1	0.94	0.10	42,42,42,42	0
56	MG	2A	3576	1/1	0.94	0.12	23,23,23,23	0
56	MG	1A	3231	1/1	0.94	0.21	53,53,53,53	0
56	MG	2A	3595	1/1	0.94	0.20	52,52,52,52	0
56	MG	1A	3486	1/1	0.94	0.08	34,34,34,34	0
56	MG	2a	3053	1/1	0.94	0.08	67,67,67,67	0
56	MG	1A	3644	1/1	0.94	0.17	41,41,41,41	0
56	MG	1a	1726	1/1	0.94	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
56	MG	1a	1610	1/1	0.94	0.10	28,28,28,28	0
56	MG	2A	3137	1/1	0.94	0.29	54,54,54,54	0
56	MG	2a	3058	1/1	0.94	0.20	53,53,53,53	0
56	MG	1A	3485	1/1	0.94	0.14	34,34,34,34	0
56	MG	2A	3507	1/1	0.94	0.13	68,68,68,68	0
56	MG	2a	3069	1/1	0.94	0.27	53,53,53,53	0
56	MG	2A	3136	1/1	0.94	0.17	24,24,24,24	0
56	MG	1n	101	1/1	0.94	0.15	45,45,45,45	0
56	MG	10	104	1/1	0.94	0.35	42,42,42,42	0
56	MG	1A	3555	1/1	0.94	0.11	35,35,35,35	0
56	MG	1a	1722	1/1	0.94	0.28	49,49,49,49	0
56	MG	2A	3273	1/1	0.94	0.24	47,47,47,47	0
56	MG	2A	3242	1/1	0.94	0.12	57,57,57,57	0
56	MG	2A	3295	1/1	0.94	0.25	38,38,38,38	0
56	MG	1A	3498	1/1	0.94	0.12	47,47,47,47	0
56	MG	1A	3847	1/1	0.94	0.10	36,36,36,36	0
56	MG	2A	3460	1/1	0.94	0.29	56,56,56,56	0
56	MG	1A	3145	1/1	0.94	0.80	53,53,53,53	0
56	MG	2A	3039	1/1	0.94	0.26	42,42,42,42	0
56	MG	2A	3539	1/1	0.94	0.45	68,68,68,68	0
56	MG	2A	3388	1/1	0.94	0.19	67,67,67,67	0
56	MG	1A	3130	1/1	0.94	0.17	54,54,54,54	0
56	MG	2A	3579	1/1	0.94	0.66	68,68,68,68	0
56	MG	1A	3442	1/1	0.94	0.25	36,36,36,36	0
56	MG	2A	3605	1/1	0.94	0.14	59,59,59,59	0
56	MG	1A	3116	1/1	0.94	0.14	44,44,44,44	0
56	MG	2A	3558	1/1	0.94	0.16	46,46,46,46	0
56	MG	1A	3120	1/1	0.94	0.28	46,46,46,46	0
56	MG	2A	3474	1/1	0.94	0.18	41,41,41,41	0
56	MG	1A	3817	1/1	0.94	0.10	47,47,47,47	0
56	MG	1A	3454	1/1	0.94	0.08	56,56,56,56	0
56	MG	1a	1678	1/1	0.94	0.38	45,45,45,45	0
56	MG	2a	3080	1/1	0.94	0.18	37,37,37,37	0
56	MG	1A	3422	1/1	0.94	0.25	27,27,27,27	0
56	MG	1A	3723	1/1	0.94	0.17	20,20,20,20	0
56	MG	2a	3051	1/1	0.94	0.17	56,56,56,56	0
56	MG	2d	301	1/1	0.94	0.24	58,58,58,58	0
56	MG	1A	3797	1/1	0.94	0.12	34,34,34,34	0
56	MG	1a	1748	1/1	0.94	0.20	49,49,49,49	0
56	MG	1A	3041	1/1	0.94	0.13	38,38,38,38	0
56	MG	1A	3262	1/1	0.94	0.14	40,40,40,40	0
56	MG	1A	3534	1/1	0.94	0.49	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3613	1/1	0.94	0.21	53,53,53,53	0
56	MG	1a	1767	1/1	0.94	0.08	47,47,47,47	0
56	MG	2A	3255	1/1	0.94	0.30	65,65,65,65	0
56	MG	1A	3324	1/1	0.94	0.52	56,56,56,56	0
56	MG	1a	1643	1/1	0.94	0.31	45,45,45,45	0
56	MG	1A	3643	1/1	0.94	0.25	34,34,34,34	0
56	MG	1A	3722	1/1	0.94	0.13	35,35,35,35	0
56	MG	1a	1654	1/1	0.94	0.27	53,53,53,53	0
56	MG	1A	3326	1/1	0.94	0.10	51,51,51,51	0
56	MG	1a	1662	1/1	0.94	0.15	37,37,37,37	0
56	MG	2A	3271	1/1	0.94	0.21	33,33,33,33	0
56	MG	1a	1721	1/1	0.94	0.24	49,49,49,49	0
56	MG	1A	3223	1/1	0.94	0.31	41,41,41,41	0
56	MG	2B	203	1/1	0.94	0.12	46,46,46,46	0
56	MG	1A	3729	1/1	0.94	0.12	52,52,52,52	0
56	MG	1A	3375	1/1	0.94	0.27	44,44,44,44	0
56	MG	1A	3824	1/1	0.94	0.25	56,56,56,56	0
56	MG	2A	3405	1/1	0.94	0.11	47,47,47,47	0
56	MG	1A	3638	1/1	0.94	0.24	64,64,64,64	0
56	MG	1A	3359	1/1	0.94	0.20	49,49,49,49	0
56	MG	1A	3682	1/1	0.94	0.07	39,39,39,39	0
56	MG	1A	3674	1/1	0.94	0.11	58,58,58,58	0
56	MG	1A	3620	1/1	0.94	0.16	29,29,29,29	0
56	MG	1A	3386	1/1	0.94	0.16	30,30,30,30	0
56	MG	1A	3728	1/1	0.94	0.09	58,58,58,58	0
56	MG	1A	3609	1/1	0.94	0.12	37,37,37,37	0
56	MG	1A	3465	1/1	0.94	0.11	26,26,26,26	0
56	MG	2a	3070	1/1	0.94	0.23	43,43,43,43	0
56	MG	1l	102	1/1	0.94	0.14	37,37,37,37	0
56	MG	1A	3666	1/1	0.94	0.11	48,48,48,48	0
56	MG	2A	3363	1/1	0.94	0.12	43,43,43,43	0
56	MG	1a	1616	1/1	0.94	0.07	53,53,53,53	0
56	MG	2A	3134	1/1	0.94	0.12	37,37,37,37	0
56	MG	1A	3126	1/1	0.94	0.14	48,48,48,48	0
56	MG	2A	3283	1/1	0.94	0.31	47,47,47,47	0
56	MG	1A	3490	1/1	0.94	0.15	28,28,28,28	0
56	MG	2A	3185	1/1	0.94	0.30	49,49,49,49	0
56	MG	1A	3719	1/1	0.94	0.20	50,50,50,50	0
56	MG	2A	3117	1/1	0.94	0.10	53,53,53,53	0
56	MG	1A	3547	1/1	0.94	0.12	47,47,47,47	0
56	MG	2A	3413	1/1	0.94	0.28	57,57,57,57	0
56	MG	1A	3398	1/1	0.94	0.35	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3474	1/1	0.94	0.13	33,33,33,33	0
56	MG	1A	3741	1/1	0.94	0.83	42,42,42,42	0
56	MG	1A	3227	1/1	0.94	0.14	34,34,34,34	0
56	MG	1A	3804	1/1	0.94	0.13	35,35,35,35	0
56	MG	1B	225	1/1	0.94	0.15	29,29,29,29	0
56	MG	1a	1750	1/1	0.94	0.11	52,52,52,52	0
56	MG	1A	3665	1/1	0.94	0.20	33,33,33,33	0
56	MG	1A	3735	1/1	0.94	0.11	56,56,56,56	0
56	MG	1a	1672	1/1	0.94	0.10	49,49,49,49	0
56	MG	2A	3164	1/1	0.94	0.12	35,35,35,35	0
56	MG	2A	3443	1/1	0.94	0.14	39,39,39,39	0
56	MG	1x	105	1/1	0.94	0.26	60,60,60,60	0
56	MG	1D	308	1/1	0.94	0.48	41,41,41,41	0
56	MG	2A	3320	1/1	0.94	0.20	45,45,45,45	0
56	MG	2A	3264	1/1	0.94	0.12	47,47,47,47	0
56	MG	1A	3340	1/1	0.94	0.11	49,49,49,49	0
56	MG	1a	1690	1/1	0.94	0.24	35,35,35,35	0
56	MG	2A	3492	1/1	0.94	0.23	69,69,69,69	0
56	MG	1A	3727	1/1	0.94	0.22	30,30,30,30	0
56	MG	1A	3703	1/1	0.95	0.12	52,52,52,52	0
56	MG	2A	3297	1/1	0.95	0.18	57,57,57,57	0
56	MG	2A	3563	1/1	0.95	0.14	59,59,59,59	0
56	MG	1A	3688	1/1	0.95	0.10	47,47,47,47	0
56	MG	2a	3022	1/1	0.95	0.23	68,68,68,68	0
56	MG	2A	3554	1/1	0.95	0.09	65,65,65,65	0
56	MG	1A	3038	1/1	0.95	0.27	43,43,43,43	0
56	MG	2A	3438	1/1	0.95	0.12	30,30,30,30	0
56	MG	1A	3537	1/1	0.95	0.13	32,32,32,32	0
56	MG	1A	3341	1/1	0.95	0.17	54,54,54,54	0
56	MG	1A	3525	1/1	0.95	0.13	25,25,25,25	0
56	MG	2a	3041	1/1	0.95	0.17	58,58,58,58	0
56	MG	1U	206	1/1	0.95	0.60	37,37,37,37	0
56	MG	2A	3178	1/1	0.95	0.30	47,47,47,47	0
56	MG	1F	307	1/1	0.95	0.80	45,45,45,45	0
56	MG	1A	3346	1/1	0.95	0.16	22,22,22,22	0
56	MG	2O	201	1/1	0.95	0.31	52,52,52,52	0
56	MG	1a	1707	1/1	0.95	0.12	37,37,37,37	0
56	MG	1a	1701	1/1	0.95	0.21	49,49,49,49	0
56	MG	2A	3075	1/1	0.95	0.18	34,34,34,34	0
56	MG	1a	1677	1/1	0.95	0.18	30,30,30,30	0
56	MG	1A	3607	1/1	0.95	0.10	35,35,35,35	0
56	MG	1A	3616	1/1	0.95	0.10	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3251	1/1	0.95	0.18	50,50,50,50	0
56	MG	1a	1716	1/1	0.95	0.32	43,43,43,43	0
56	MG	2A	3407	1/1	0.95	0.08	75,75,75,75	0
56	MG	2A	3452	1/1	0.95	0.19	48,48,48,48	0
56	MG	1A	3585	1/1	0.95	0.12	50,50,50,50	0
56	MG	2a	3040	1/1	0.95	0.13	50,50,50,50	0
56	MG	2A	3520	1/1	0.95	0.12	39,39,39,39	0
56	MG	1A	3798	1/1	0.95	0.14	27,27,27,27	0
56	MG	1A	3091	1/1	0.95	0.59	39,39,39,39	0
56	MG	1a	1704	1/1	0.95	0.25	41,41,41,41	0
56	MG	2A	3505	1/1	0.95	0.27	59,59,59,59	0
56	MG	1A	3144	1/1	0.95	0.10	34,34,34,34	0
56	MG	1U	204	1/1	0.95	0.44	43,43,43,43	0
56	MG	1W	203	1/1	0.95	0.12	48,48,48,48	0
56	MG	2A	3546	1/1	0.95	0.12	59,59,59,59	0
56	MG	1A	3237	1/1	0.95	0.11	45,45,45,45	0
56	MG	1A	3299	1/1	0.95	0.12	31,31,31,31	0
56	MG	1A	3739	1/1	0.95	0.34	66,66,66,66	0
56	MG	1A	3245	1/1	0.95	0.50	41,41,41,41	0
56	MG	1A	3225	1/1	0.95	0.24	35,35,35,35	0
56	MG	2A	3284	1/1	0.95	0.23	47,47,47,47	0
56	MG	1A	3496	1/1	0.95	0.10	58,58,58,58	0
56	MG	2A	3449	1/1	0.95	0.11	61,61,61,61	0
56	MG	1A	3592	1/1	0.95	0.16	27,27,27,27	0
56	MG	1A	3011	1/1	0.95	0.18	31,31,31,31	0
56	MG	2A	3437	1/1	0.95	0.19	33,33,33,33	0
56	MG	1A	3046	1/1	0.95	0.14	46,46,46,46	0
56	MG	2A	3620	1/1	0.95	0.11	61,61,61,61	0
56	MG	28	102	1/1	0.95	0.13	48,48,48,48	0
56	MG	2A	3586	1/1	0.95	0.09	50,50,50,50	0
56	MG	2A	3188	1/1	0.95	0.15	56,56,56,56	0
56	MG	1F	306	1/1	0.95	0.29	47,47,47,47	0
56	MG	1A	3536	1/1	0.95	0.24	63,63,63,63	0
56	MG	2A	3027	1/1	0.95	0.20	34,34,34,34	0
56	MG	1A	3328	1/1	0.95	0.21	34,34,34,34	0
56	MG	2a	3137	1/1	0.95	0.13	58,58,58,58	0
56	MG	1a	1669	1/1	0.95	0.21	38,38,38,38	0
56	MG	2A	3544	1/1	0.95	0.10	54,54,54,54	0
56	MG	2A	3004	1/1	0.95	0.09	48,48,48,48	0
56	MG	2A	3263	1/1	0.95	0.26	51,51,51,51	0
56	MG	2A	3500	1/1	0.95	0.11	58,58,58,58	0
56	MG	1A	3505	1/1	0.95	0.22	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3412	1/1	0.95	0.25	28,28,28,28	0
56	MG	1A	3406	1/1	0.95	0.55	57,57,57,57	0
56	MG	1W	205	1/1	0.95	0.41	38,38,38,38	0
56	MG	27	102	1/1	0.95	0.47	42,42,42,42	0
56	MG	2a	3013	1/1	0.95	0.12	56,56,56,56	0
56	MG	1E	303	1/1	0.95	0.16	33,33,33,33	0
56	MG	1x	109	1/1	0.95	0.21	60,60,60,60	0
56	MG	1A	3751	1/1	0.95	0.21	53,53,53,53	0
56	MG	2A	3584	1/1	0.95	0.20	78,78,78,78	0
56	MG	2A	3498	1/1	0.95	0.11	50,50,50,50	0
56	MG	1A	3594	1/1	0.95	0.12	64,64,64,64	0
56	MG	1A	3196	1/1	0.95	0.11	44,44,44,44	0
56	MG	2B	202	1/1	0.95	0.15	57,57,57,57	0
56	MG	1A	3067	1/1	0.95	0.23	40,40,40,40	0
56	MG	1A	3499	1/1	0.95	0.13	23,23,23,23	0
56	MG	1G	203	1/1	0.95	0.09	53,53,53,53	0
56	MG	2A	3463	1/1	0.95	0.17	47,47,47,47	0
56	MG	1A	3507	1/1	0.95	0.23	38,38,38,38	0
56	MG	1a	1760	1/1	0.95	0.23	37,37,37,37	0
56	MG	1A	3357	1/1	0.95	0.14	26,26,26,26	0
56	MG	2A	3349	1/1	0.95	0.11	33,33,33,33	0
56	MG	2A	3581	1/1	0.95	0.15	81,81,81,81	0
56	MG	1A	3670	1/1	0.95	0.09	38,38,38,38	0
56	MG	2A	3448	1/1	0.95	0.15	51,51,51,51	0
56	MG	1A	3736	1/1	0.95	0.09	35,35,35,35	0
56	MG	1A	3538	1/1	0.95	0.11	33,33,33,33	0
56	MG	1a	1612	1/1	0.95	0.26	45,45,45,45	0
56	MG	2a	3042	1/1	0.95	0.09	51,51,51,51	0
56	MG	2A	3322	1/1	0.95	0.17	44,44,44,44	0
56	MG	2A	3490	1/1	0.95	0.16	47,47,47,47	0
56	MG	1F	303	1/1	0.95	0.66	36,36,36,36	0
56	MG	1A	3840	1/1	0.95	0.13	59,59,59,59	0
56	MG	17	3104	1/1	0.95	0.65	39,39,39,39	0
56	MG	2A	3482	1/1	0.95	0.18	52,52,52,52	0
56	MG	1A	3823	1/1	0.95	0.20	46,46,46,46	0
56	MG	1U	201	1/1	0.95	0.60	42,42,42,42	0
56	MG	1A	3272	1/1	0.95	0.23	42,42,42,42	0
56	MG	1A	3138	1/1	0.95	0.13	36,36,36,36	0
56	MG	2A	3590	1/1	0.95	0.16	49,49,49,49	0
56	MG	2a	3026	1/1	0.95	0.12	54,54,54,54	0
56	MG	2A	3091	1/1	0.95	0.13	34,34,34,34	0
56	MG	1E	306	1/1	0.95	0.43	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1d	301	1/1	0.95	0.20	57,57,57,57	0
56	MG	2x	104	1/1	0.95	0.24	41,41,41,41	0
56	MG	2A	3503	1/1	0.95	0.20	41,41,41,41	0
56	MG	2A	3511	1/1	0.95	0.11	37,37,37,37	0
56	MG	2A	3269	1/1	0.95	0.16	26,26,26,26	0
56	MG	1A	3780	1/1	0.95	0.14	64,64,64,64	0
56	MG	2A	3542	1/1	0.95	0.11	50,50,50,50	0
56	MG	2a	3005	1/1	0.95	0.23	52,52,52,52	0
56	MG	1A	3495	1/1	0.95	0.09	49,49,49,49	0
56	MG	1A	3567	1/1	0.95	0.17	59,59,59,59	0
56	MG	1A	3701	1/1	0.95	0.08	47,47,47,47	0
56	MG	1A	3473	1/1	0.95	0.07	26,26,26,26	0
56	MG	1A	3672	1/1	0.95	0.10	46,46,46,46	0
56	MG	2A	3205	1/1	0.95	0.18	40,40,40,40	0
56	MG	1A	3009	1/1	0.95	0.09	33,33,33,33	0
56	MG	1A	3603	1/1	0.95	0.14	55,55,55,55	0
56	MG	1A	3387	1/1	0.95	0.62	42,42,42,42	0
56	MG	2A	3619	1/1	0.95	0.12	35,35,35,35	0
56	MG	1A	3503	1/1	0.95	0.16	49,49,49,49	0
56	MG	1a	1729	1/1	0.95	0.29	38,38,38,38	0
56	MG	1A	3721	1/1	0.95	0.14	35,35,35,35	0
56	MG	1a	1609	1/1	0.95	0.13	41,41,41,41	0
56	MG	1A	3048	1/1	0.95	0.15	50,50,50,50	0
56	MG	1A	3695	1/1	0.95	0.18	42,42,42,42	0
56	MG	1A	3456	1/1	0.95	0.30	49,49,49,49	0
56	MG	2A	3423	1/1	0.95	0.24	34,34,34,34	0
56	MG	1A	3409	1/1	0.95	0.16	38,38,38,38	0
56	MG	1A	3061	1/1	0.95	0.20	32,32,32,32	0
56	MG	2A	3571	1/1	0.95	0.10	53,53,53,53	0
56	MG	1A	3308	1/1	0.95	0.17	47,47,47,47	0
56	MG	1A	3381	1/1	0.95	0.14	45,45,45,45	0
56	MG	2A	3132	1/1	0.95	0.17	58,58,58,58	0
56	MG	2A	3193	1/1	0.95	0.25	45,45,45,45	0
56	MG	1a	1622	1/1	0.95	0.18	32,32,32,32	0
56	MG	1a	1619	1/1	0.95	0.23	53,53,53,53	0
56	MG	2A	3568	1/1	0.95	0.10	64,64,64,64	0
56	MG	1A	3531	1/1	0.95	0.15	46,46,46,46	0
56	MG	1A	3029	1/1	0.95	0.35	47,47,47,47	0
56	MG	1A	3600	1/1	0.95	0.06	60,60,60,60	0
56	MG	2A	3575	1/1	0.95	0.18	48,48,48,48	0
56	MG	1B	217	1/1	0.95	0.14	43,43,43,43	0
56	MG	1a	1652	1/1	0.95	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
56	MG	1A	3588	1/1	0.95	0.14	41,41,41,41	0
56	MG	2A	3215	1/1	0.95	0.28	60,60,60,60	0
56	MG	25	101	1/1	0.95	0.12	43,43,43,43	0
56	MG	1A	3133	1/1	0.95	0.08	31,31,31,31	0
56	MG	2A	3352	1/1	0.95	0.11	44,44,44,44	0
56	MG	1A	3459	1/1	0.95	0.24	25,25,25,25	0
56	MG	1A	3119	1/1	0.95	0.23	44,44,44,44	0
56	MG	2a	3122	1/1	0.95	0.21	65,65,65,65	0
56	MG	2A	3551	1/1	0.95	0.69	57,57,57,57	0
56	MG	1A	3471	1/1	0.95	0.14	44,44,44,44	0
56	MG	2A	3353	1/1	0.95	0.15	30,30,30,30	0
56	MG	1A	3220	1/1	0.95	0.31	48,48,48,48	0
56	MG	2A	3446	1/1	0.95	0.13	35,35,35,35	0
56	MG	1A	3590	1/1	0.95	0.08	56,56,56,56	0
56	MG	2A	3265	1/1	0.95	0.10	53,53,53,53	0
56	MG	1A	3377	1/1	0.95	0.14	61,61,61,61	0
56	MG	2F	304	1/1	0.95	0.26	56,56,56,56	0
56	MG	1A	3115	1/1	0.95	0.14	31,31,31,31	0
56	MG	1A	3750	1/1	0.95	0.14	58,58,58,58	0
56	MG	1B	201	1/1	0.95	0.14	31,31,31,31	0
56	MG	1A	3092	1/1	0.95	0.13	36,36,36,36	0
56	MG	2B	211	1/1	0.95	0.28	54,54,54,54	0
56	MG	1A	3256	1/1	0.95	0.29	49,49,49,49	0
56	MG	1A	3206	1/1	0.95	0.20	32,32,32,32	0
56	MG	2A	3427	1/1	0.95	0.24	42,42,42,42	0
56	MG	25	102	1/1	0.95	0.18	50,50,50,50	0
56	MG	2A	3557	1/1	0.95	0.09	47,47,47,47	0
56	MG	1A	3694	1/1	0.95	0.10	40,40,40,40	0
56	MG	1a	1613	1/1	0.95	0.11	51,51,51,51	0
56	MG	1A	3812	1/1	0.95	0.09	26,26,26,26	0
56	MG	1A	3686	1/1	0.95	0.08	61,61,61,61	0
56	MG	2A	3001	1/1	0.95	0.13	35,35,35,35	0
56	MG	1a	1641	1/1	0.95	0.12	57,57,57,57	0
56	MG	1A	3730	1/1	0.96	0.11	39,39,39,39	0
56	MG	1a	1689	1/1	0.96	0.18	48,48,48,48	0
56	MG	1A	3458	1/1	0.96	0.14	45,45,45,45	0
56	MG	1A	3348	1/1	0.96	0.24	34,34,34,34	0
56	MG	1a	1651	1/1	0.96	0.18	44,44,44,44	0
56	MG	2A	3321	1/1	0.96	0.19	35,35,35,35	0
56	MG	2A	3418	1/1	0.96	0.17	37,37,37,37	0
56	MG	2A	3521	1/1	0.96	0.10	60,60,60,60	0
56	MG	1P	204	1/1	0.96	0.54	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3642	1/1	0.96	0.08	21,21,21,21	0
56	MG	1a	1693	1/1	0.96	0.19	34,34,34,34	0
56	MG	1A	3127	1/1	0.96	0.28	52,52,52,52	0
56	MG	1A	3329	1/1	0.96	0.11	34,34,34,34	0
56	MG	2A	3291	1/1	0.96	0.17	43,43,43,43	0
56	MG	1A	3711	1/1	0.96	0.41	42,42,42,42	0
56	MG	2A	3621	1/1	0.96	0.09	58,58,58,58	0
56	MG	1A	3775	1/1	0.96	0.12	54,54,54,54	0
56	MG	1B	222	1/1	0.96	0.14	47,47,47,47	0
56	MG	2A	3316	1/1	0.96	0.19	44,44,44,44	0
56	MG	2A	3163	1/1	0.96	0.29	30,30,30,30	0
56	MG	2A	3535	1/1	0.96	0.30	54,54,54,54	0
56	MG	2A	3624	1/1	0.96	0.16	34,34,34,34	0
56	MG	1A	3044	1/1	0.96	0.18	35,35,35,35	0
56	MG	2A	3162	1/1	0.96	0.28	68,68,68,68	0
56	MG	2A	3290	1/1	0.96	0.20	36,36,36,36	0
56	MG	1W	201	1/1	0.96	0.33	35,35,35,35	0
56	MG	1A	3501	1/1	0.96	0.11	58,58,58,58	0
56	MG	1R	202	1/1	0.96	0.42	52,52,52,52	0
56	MG	2a	3127	1/1	0.96	0.08	65,65,65,65	0
56	MG	1A	3131	1/1	0.96	0.28	32,32,32,32	0
56	MG	1A	3506	1/1	0.96	0.12	41,41,41,41	0
56	MG	1a	1700	1/1	0.96	0.28	24,24,24,24	0
56	MG	1A	3845	1/1	0.96	0.22	47,47,47,47	0
56	MG	1a	1645	1/1	0.96	0.09	35,35,35,35	0
56	MG	2A	3472	1/1	0.96	0.12	33,33,33,33	0
56	MG	1a	1601	1/1	0.96	0.26	61,61,61,61	0
56	MG	2A	3525	1/1	0.96	0.15	45,45,45,45	0
56	MG	2A	3194	1/1	0.96	0.64	43,43,43,43	0
56	MG	1e	202	1/1	0.96	0.18	47,47,47,47	0
56	MG	2A	3600	1/1	0.96	0.24	43,43,43,43	0
56	MG	1A	3446	1/1	0.96	0.25	22,22,22,22	0
56	MG	2A	3097	1/1	0.96	0.18	54,54,54,54	0
56	MG	2a	3012	1/1	0.96	0.12	52,52,52,52	0
56	MG	1A	3197	1/1	0.96	0.22	43,43,43,43	0
56	MG	2A	3086	1/1	0.96	0.20	36,36,36,36	0
56	MG	1A	3510	1/1	0.96	0.15	33,33,33,33	0
56	MG	2A	3029	1/1	0.96	0.12	38,38,38,38	0
56	MG	2A	3191	1/1	0.96	0.18	50,50,50,50	0
56	MG	1A	3743	1/1	0.96	0.08	33,33,33,33	0
56	MG	1a	1685	1/1	0.96	0.09	53,53,53,53	0
56	MG	2A	3033	1/1	0.96	0.10	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1a	1684	1/1	0.96	0.12	51,51,51,51	0
56	MG	1A	3288	1/1	0.96	0.11	52,52,52,52	0
56	MG	2a	3093	1/1	0.96	0.13	50,50,50,50	0
56	MG	2A	3150	1/1	0.96	0.12	51,51,51,51	0
56	MG	1A	3586	1/1	0.96	0.18	44,44,44,44	0
56	MG	1A	3097	1/1	0.96	0.34	38,38,38,38	0
56	MG	2B	212	1/1	0.96	0.24	49,49,49,49	0
56	MG	2A	3623	1/1	0.96	0.10	39,39,39,39	0
56	MG	1A	3788	1/1	0.96	0.13	33,33,33,33	0
56	MG	1A	3601	1/1	0.96	0.10	36,36,36,36	0
56	MG	2A	3501	1/1	0.96	0.08	42,42,42,42	0
56	MG	1A	3645	1/1	0.96	0.18	50,50,50,50	0
56	MG	2A	3068	1/1	0.96	0.19	44,44,44,44	0
56	MG	2a	3004	1/1	0.96	0.08	60,60,60,60	0
56	MG	1R	206	1/1	0.96	0.13	34,34,34,34	0
56	MG	1a	1630	1/1	0.96	0.12	38,38,38,38	0
56	MG	2A	3116	1/1	0.96	0.17	49,49,49,49	0
56	MG	1A	3204	1/1	0.96	0.28	25,25,25,25	0
56	MG	2A	3508	1/1	0.96	0.19	53,53,53,53	0
56	MG	1A	3069	1/1	0.96	0.11	36,36,36,36	0
56	MG	1U	203	1/1	0.96	0.59	41,41,41,41	0
56	MG	1A	3646	1/1	0.96	0.29	56,56,56,56	0
56	MG	1A	3677	1/1	0.96	0.09	50,50,50,50	0
56	MG	1A	3838	1/1	0.96	0.11	36,36,36,36	0
56	MG	1A	3017	1/1	0.96	0.10	37,37,37,37	0
56	MG	1a	1725	1/1	0.96	0.09	67,67,67,67	0
56	MG	1F	310	1/1	0.96	0.64	31,31,31,31	0
56	MG	1A	3251	1/1	0.96	0.10	48,48,48,48	0
56	MG	1A	3550	1/1	0.96	0.12	31,31,31,31	0
56	MG	2A	3493	1/1	0.96	0.22	45,45,45,45	0
56	MG	2A	3456	1/1	0.96	0.16	39,39,39,39	0
56	MG	2A	3053	1/1	0.96	0.22	53,53,53,53	0
56	MG	2A	3597	1/1	0.96	0.20	49,49,49,49	0
56	MG	2A	3046	1/1	0.96	0.09	36,36,36,36	0
56	MG	1A	3563	1/1	0.96	0.29	57,57,57,57	0
56	MG	2A	3228	1/1	0.96	0.31	45,45,45,45	0
56	MG	1A	3362	1/1	0.96	0.25	46,46,46,46	0
56	MG	2a	3075	1/1	0.96	0.16	39,39,39,39	0
56	MG	1A	3235	1/1	0.96	0.11	15,15,15,15	0
56	MG	1A	3746	1/1	0.96	0.54	48,48,48,48	0
56	MG	1A	3254	1/1	0.96	0.29	64,64,64,64	0
56	MG	1a	1671	1/1	0.96	0.21	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3045	1/1	0.96	0.21	47,47,47,47	0
56	MG	2A	3209	1/1	0.96	0.10	63,63,63,63	0
56	MG	2a	3045	1/1	0.96	0.12	49,49,49,49	0
56	MG	2A	3524	1/1	0.96	0.14	55,55,55,55	0
56	MG	2A	3087	1/1	0.96	0.25	53,53,53,53	0
56	MG	1A	3163	1/1	0.96	0.54	38,38,38,38	0
56	MG	1A	3057	1/1	0.96	0.18	20,20,20,20	0
57	ZN	14	102	1/1	0.96	0.11	88,88,88,88	0
56	MG	1A	3523	1/1	0.96	0.07	35,35,35,35	0
56	MG	1A	3268	1/1	0.96	0.20	43,43,43,43	0
56	MG	1A	3140	1/1	0.96	0.11	37,37,37,37	0
56	MG	1a	1611	1/1	0.96	0.15	49,49,49,49	0
56	MG	1A	3828	1/1	0.96	0.14	40,40,40,40	0
56	MG	2A	3041	1/1	0.96	0.10	35,35,35,35	0
56	MG	1A	3676	1/1	0.96	0.86	67,67,67,67	0
56	MG	2A	3598	1/1	0.96	0.16	49,49,49,49	0
56	MG	2A	3124	1/1	0.96	0.22	47,47,47,47	0
56	MG	1R	205	1/1	0.96	0.15	29,29,29,29	0
56	MG	1A	3683	1/1	0.96	0.15	55,55,55,55	0
56	MG	1D	305	1/1	0.96	0.23	43,43,43,43	0
56	MG	2a	3067	1/1	0.96	0.10	58,58,58,58	0
56	MG	2A	3517	1/1	0.96	0.10	49,49,49,49	0
56	MG	2a	3141	1/1	0.96	0.08	46,46,46,46	0
56	MG	1Z	303	1/1	0.96	0.12	35,35,35,35	0
56	MG	1A	3689	1/1	0.96	0.17	43,43,43,43	0
56	MG	1B	218	1/1	0.96	0.32	52,52,52,52	0
56	MG	2A	3567	1/1	0.96	0.10	51,51,51,51	0
56	MG	1A	3202	1/1	0.96	0.30	38,38,38,38	0
56	MG	2a	3068	1/1	0.96	0.21	48,48,48,48	0
56	MG	2A	3475	1/1	0.96	0.20	35,35,35,35	0
56	MG	1A	3420	1/1	0.96	0.33	41,41,41,41	0
56	MG	1A	3121	1/1	0.96	0.18	22,22,22,22	0
56	MG	2A	3231	1/1	0.96	0.38	50,50,50,50	0
56	MG	1a	1698	1/1	0.96	0.21	42,42,42,42	0
56	MG	2A	3050	1/1	0.96	0.11	30,30,30,30	0
56	MG	2A	3534	1/1	0.96	0.12	36,36,36,36	0
56	MG	2A	3433	1/1	0.96	0.14	47,47,47,47	0
56	MG	2A	3536	1/1	0.96	0.09	35,35,35,35	0
56	MG	1a	1674	1/1	0.96	0.18	48,48,48,48	0
56	MG	2A	3533	1/1	0.96	0.14	44,44,44,44	0
56	MG	1A	3502	1/1	0.96	0.24	30,30,30,30	0
56	MG	1Z	302	1/1	0.96	0.11	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3210	1/1	0.96	0.12	76,76,76,76	0
57	ZN	2Y	202	1/1	0.96	0.13	76,76,76,76	0
56	MG	1x	103	1/1	0.96	0.23	55,55,55,55	0
56	MG	2A	3362	1/1	0.96	0.18	30,30,30,30	0
56	MG	1A	3562	1/1	0.96	0.14	61,61,61,61	0
56	MG	1A	3574	1/1	0.96	0.16	61,61,61,61	0
56	MG	2A	3562	1/1	0.96	0.17	53,53,53,53	0
56	MG	1X	101	1/1	0.96	0.20	35,35,35,35	0
56	MG	1A	3811	1/1	0.96	0.15	17,17,17,17	0
56	MG	1A	3532	1/1	0.96	0.09	22,22,22,22	0
56	MG	1A	3323	1/1	0.96	0.66	48,48,48,48	0
56	MG	2a	3008	1/1	0.96	0.29	46,46,46,46	0
56	MG	1R	201	1/1	0.96	0.34	42,42,42,42	0
56	MG	2A	3252	1/1	0.96	0.23	38,38,38,38	0
56	MG	2A	3309	1/1	0.96	0.09	65,65,65,65	0
56	MG	1A	3744	1/1	0.96	0.21	22,22,22,22	0
56	MG	1A	3095	1/1	0.96	0.24	37,37,37,37	0
56	MG	1A	3443	1/1	0.96	0.19	33,33,33,33	0
56	MG	1A	3122	1/1	0.96	0.11	27,27,27,27	0
56	MG	1A	3450	1/1	0.96	0.14	34,34,34,34	0
56	MG	2A	3202	1/1	0.96	0.33	44,44,44,44	0
56	MG	1a	1632	1/1	0.96	0.14	49,49,49,49	0
56	MG	2A	3445	1/1	0.96	0.30	48,48,48,48	0
56	MG	1a	1687	1/1	0.96	0.20	37,37,37,37	0
56	MG	1A	3330	1/1	0.96	0.44	48,48,48,48	0
56	MG	1a	1656	1/1	0.96	0.12	44,44,44,44	0
56	MG	2A	3110	1/1	0.96	0.10	49,49,49,49	0
56	MG	2A	3470	1/1	0.96	0.10	39,39,39,39	0
56	MG	1A	3542	1/1	0.96	0.13	36,36,36,36	0
56	MG	1A	3405	1/1	0.96	0.11	43,43,43,43	0
56	MG	1Y	201	1/1	0.96	0.08	61,61,61,61	0
56	MG	2A	3198	1/1	0.96	0.26	47,47,47,47	0
56	MG	2A	3013	1/1	0.96	0.11	24,24,24,24	0
56	MG	1A	3818	1/1	0.96	0.16	28,28,28,28	0
56	MG	1A	3008	1/1	0.96	0.11	22,22,22,22	0
56	MG	2a	3143	1/1	0.96	0.10	49,49,49,49	0
56	MG	1G	204	1/1	0.96	0.27	44,44,44,44	0
56	MG	1A	3010	1/1	0.96	0.09	42,42,42,42	0
56	MG	1A	3066	1/1	0.96	0.24	39,39,39,39	0
56	MG	1A	3733	1/1	0.96	0.21	34,34,34,34	0
56	MG	2A	3430	1/1	0.96	0.19	20,20,20,20	0
56	MG	2a	3129	1/1	0.96	0.06	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1a	1642	1/1	0.96	0.21	41,41,41,41	0
56	MG	1A	3207	1/1	0.96	0.13	26,26,26,26	0
56	MG	1A	3629	1/1	0.96	0.34	54,54,54,54	0
56	MG	2A	3424	1/1	0.96	0.27	43,43,43,43	0
56	MG	1W	206	1/1	0.96	0.32	25,25,25,25	0
56	MG	2A	3608	1/1	0.96	0.09	37,37,37,37	0
56	MG	1A	3425	1/1	0.96	0.15	24,24,24,24	0
56	MG	2A	3115	1/1	0.96	0.08	53,53,53,53	0
56	MG	1A	3063	1/1	0.96	0.19	32,32,32,32	0
56	MG	1A	3385	1/1	0.96	0.61	38,38,38,38	0
56	MG	15	104	1/1	0.96	0.15	44,44,44,44	0
56	MG	1B	212	1/1	0.96	0.37	51,51,51,51	0
56	MG	1A	3487	1/1	0.96	0.12	47,47,47,47	0
56	MG	2A	3071	1/1	0.96	0.34	46,46,46,46	0
56	MG	13	101	1/1	0.96	0.19	42,42,42,42	0
56	MG	2A	3359	1/1	0.96	0.22	52,52,52,52	0
56	MG	1a	1747	1/1	0.96	0.26	46,46,46,46	0
56	MG	2A	3247	1/1	0.96	0.24	50,50,50,50	0
56	MG	2A	3444	1/1	0.96	0.18	34,34,34,34	0
56	MG	2A	3292	1/1	0.96	0.21	32,32,32,32	0
56	MG	1A	3293	1/1	0.96	0.16	41,41,41,41	0
56	MG	2A	3331	1/1	0.96	0.16	42,42,42,42	0
56	MG	1A	3166	1/1	0.96	0.16	40,40,40,40	0
56	MG	2R	201	1/1	0.96	0.13	31,31,31,31	0
56	MG	2A	3130	1/1	0.96	0.14	29,29,29,29	0
56	MG	2A	3223	1/1	0.96	0.12	37,37,37,37	0
56	MG	2A	3319	1/1	0.96	0.13	51,51,51,51	0
56	MG	2A	3256	1/1	0.96	0.32	46,46,46,46	0
56	MG	2k	201	1/1	0.96	0.07	63,63,63,63	0
56	MG	1A	3732	1/1	0.96	0.12	40,40,40,40	0
56	MG	1Q	203	1/1	0.96	0.22	24,24,24,24	0
56	MG	2A	3383	1/1	0.96	0.23	25,25,25,25	0
56	MG	1A	3401	1/1	0.96	0.21	55,55,55,55	0
56	MG	2P	203	1/1	0.96	0.17	60,60,60,60	0
56	MG	1F	312	1/1	0.96	0.15	46,46,46,46	0
56	MG	1A	3478	1/1	0.96	0.14	52,52,52,52	0
56	MG	1A	3820	1/1	0.96	0.23	41,41,41,41	0
56	MG	1A	3581	1/1	0.96	0.09	28,28,28,28	0
56	MG	2A	3047	1/1	0.96	0.28	52,52,52,52	0
56	MG	2A	3390	1/1	0.96	0.10	46,46,46,46	0
56	MG	2A	3012	1/1	0.96	0.14	47,47,47,47	0
56	MG	1a	1761	1/1	0.96	0.34	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3831	1/1	0.96	0.18	71,71,71,71	0
56	MG	2A	3221	1/1	0.96	0.19	42,42,42,42	0
56	MG	1A	3599	1/1	0.96	0.16	59,59,59,59	0
56	MG	1A	3141	1/1	0.96	0.18	41,41,41,41	0
56	MG	2A	3199	1/1	0.96	0.14	46,46,46,46	0
56	MG	1A	3690	1/1	0.96	0.10	58,58,58,58	0
56	MG	1A	3787	1/1	0.96	0.19	42,42,42,42	0
56	MG	1a	1754	1/1	0.96	0.12	49,49,49,49	0
56	MG	2A	3088	1/1	0.96	0.33	35,35,35,35	0
56	MG	2A	3037	1/1	0.96	0.16	50,50,50,50	0
56	MG	1A	3393	1/1	0.96	0.18	40,40,40,40	0
56	MG	1A	3591	1/1	0.96	0.15	46,46,46,46	0
56	MG	2A	3076	1/1	0.96	0.10	43,43,43,43	0
56	MG	2A	3420	1/1	0.96	0.20	42,42,42,42	0
56	MG	15	105	1/1	0.96	0.15	37,37,37,37	0
56	MG	1A	3813	1/1	0.96	0.13	36,36,36,36	0
56	MG	2A	3107	1/1	0.96	0.24	51,51,51,51	0
56	MG	2A	3553	1/1	0.96	0.11	62,62,62,62	0
56	MG	1E	301	1/1	0.96	0.13	49,49,49,49	0
56	MG	2A	3391	1/1	0.96	0.14	94,94,94,94	0
56	MG	2A	3056	1/1	0.96	0.06	52,52,52,52	0
56	MG	1A	3047	1/1	0.96	0.29	49,49,49,49	0
56	MG	2a	3019	1/1	0.96	0.14	55,55,55,55	0
56	MG	1A	3608	1/1	0.97	0.21	32,32,32,32	0
56	MG	2A	3440	1/1	0.97	0.28	38,38,38,38	0
56	MG	1A	3424	1/1	0.97	0.26	31,31,31,31	0
56	MG	1a	1746	1/1	0.97	0.15	34,34,34,34	0
56	MG	2A	3347	1/1	0.97	0.31	28,28,28,28	0
56	MG	1A	3447	1/1	0.97	0.23	47,47,47,47	0
56	MG	1A	3491	1/1	0.97	0.10	25,25,25,25	0
56	MG	1A	3809	1/1	0.97	0.09	46,46,46,46	0
56	MG	2a	3077	1/1	0.97	0.17	46,46,46,46	0
56	MG	2a	3066	1/1	0.97	0.11	48,48,48,48	0
56	MG	1X	102	1/1	0.97	0.22	58,58,58,58	0
56	MG	2A	3216	1/1	0.97	0.16	41,41,41,41	0
56	MG	2A	3072	1/1	0.97	0.40	54,54,54,54	0
56	MG	2A	3494	1/1	0.97	0.10	50,50,50,50	0
56	MG	2A	3457	1/1	0.97	0.17	60,60,60,60	0
56	MG	2Q	201	1/1	0.97	0.12	57,57,57,57	0
56	MG	1x	101	1/1	0.97	0.23	26,26,26,26	0
56	MG	1A	3093	1/1	0.97	0.16	41,41,41,41	0
56	MG	1a	1638	1/1	0.97	0.10	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3832	1/1	0.97	0.24	54,54,54,54	0
56	MG	1A	3548	1/1	0.97	0.30	29,29,29,29	0
56	MG	1A	3681	1/1	0.97	0.05	57,57,57,57	0
56	MG	1A	3167	1/1	0.97	0.09	63,63,63,63	0
56	MG	2A	3513	1/1	0.97	0.15	57,57,57,57	0
56	MG	2E	302	1/1	0.97	0.12	29,29,29,29	0
56	MG	1D	303	1/1	0.97	0.28	55,55,55,55	0
56	MG	2A	3240	1/1	0.97	0.27	41,41,41,41	0
56	MG	2A	3545	1/1	0.97	0.16	53,53,53,53	0
56	MG	2A	3480	1/1	0.97	0.12	36,36,36,36	0
56	MG	1A	3242	1/1	0.97	0.23	43,43,43,43	0
56	MG	1A	3099	1/1	0.97	0.15	26,26,26,26	0
56	MG	2A	3479	1/1	0.97	0.14	36,36,36,36	0
56	MG	2A	3227	1/1	0.97	0.10	28,28,28,28	0
56	MG	2A	3451	1/1	0.97	0.17	45,45,45,45	0
56	MG	2A	3481	1/1	0.97	0.09	47,47,47,47	0
56	MG	1A	3476	1/1	0.97	0.17	33,33,33,33	0
56	MG	2A	3371	1/1	0.97	0.18	34,34,34,34	0
56	MG	1A	3835	1/1	0.97	0.13	48,48,48,48	0
56	MG	2A	3417	1/1	0.97	0.11	27,27,27,27	0
56	MG	1A	3429	1/1	0.97	0.26	31,31,31,31	0
56	MG	2A	3246	1/1	0.97	0.10	45,45,45,45	0
56	MG	1A	3001	1/1	0.97	0.19	39,39,39,39	0
56	MG	1A	3783	1/1	0.97	0.11	32,32,32,32	0
56	MG	2A	3177	1/1	0.97	0.16	53,53,53,53	0
56	MG	1A	3304	1/1	0.97	0.13	41,41,41,41	0
56	MG	2A	3149	1/1	0.97	0.18	55,55,55,55	0
56	MG	1A	3769	1/1	0.97	0.05	52,52,52,52	0
56	MG	2A	3453	1/1	0.97	0.12	35,35,35,35	0
56	MG	2A	3298	1/1	0.97	0.24	44,44,44,44	0
56	MG	1v	101	1/1	0.97	0.20	41,41,41,41	0
56	MG	2A	3381	1/1	0.97	0.11	44,44,44,44	0
56	MG	1A	3426	1/1	0.97	0.41	29,29,29,29	0
56	MG	1A	3700	1/1	0.97	0.07	47,47,47,47	0
56	MG	2A	3612	1/1	0.97	0.09	42,42,42,42	0
56	MG	1A	3477	1/1	0.97	0.18	35,35,35,35	0
56	MG	1A	3552	1/1	0.97	0.15	14,14,14,14	0
56	MG	1A	3104	1/1	0.97	0.07	54,54,54,54	0
56	MG	1a	1762	1/1	0.97	0.14	50,50,50,50	0
56	MG	2A	3300	1/1	0.97	0.20	29,29,29,29	0
56	MG	2A	3157	1/1	0.97	0.10	57,57,57,57	0
56	MG	1A	3647	1/1	0.97	0.22	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3285	1/1	0.97	0.16	36,36,36,36	0
56	MG	1A	3612	1/1	0.97	0.09	34,34,34,34	0
56	MG	1a	1703	1/1	0.97	0.23	48,48,48,48	0
56	MG	1A	3668	1/1	0.97	0.15	37,37,37,37	0
56	MG	1A	3411	1/1	0.97	0.09	54,54,54,54	0
56	MG	1A	3022	1/1	0.97	0.12	29,29,29,29	0
56	MG	1A	3294	1/1	0.97	0.14	27,27,27,27	0
56	MG	2A	3120	1/1	0.97	0.18	39,39,39,39	0
56	MG	2A	3081	1/1	0.97	0.30	57,57,57,57	0
56	MG	2A	3108	1/1	0.97	0.15	55,55,55,55	0
56	MG	1A	3573	1/1	0.97	0.27	53,53,53,53	0
56	MG	1F	304	1/1	0.97	0.50	38,38,38,38	0
56	MG	18	101	1/1	0.97	0.37	39,39,39,39	0
56	MG	1A	3561	1/1	0.97	0.17	26,26,26,26	0
56	MG	2A	3062	1/1	0.97	0.10	47,47,47,47	0
56	MG	2Q	202	1/1	0.97	0.17	33,33,33,33	0
56	MG	1A	3012	1/1	0.97	0.24	38,38,38,38	0
56	MG	2a	3046	1/1	0.97	0.18	49,49,49,49	0
56	MG	2A	3287	1/1	0.97	0.24	38,38,38,38	0
56	MG	2a	3130	1/1	0.97	0.12	53,53,53,53	0
56	MG	2E	305	1/1	0.97	0.15	32,32,32,32	0
56	MG	2A	3532	1/1	0.97	0.10	46,46,46,46	0
56	MG	1A	3610	1/1	0.97	0.12	35,35,35,35	0
56	MG	1A	3650	1/1	0.97	0.16	29,29,29,29	0
56	MG	2A	3496	1/1	0.97	0.11	41,41,41,41	0
56	MG	2A	3596	1/1	0.97	0.17	50,50,50,50	0
56	MG	2A	3502	1/1	0.97	0.10	40,40,40,40	0
56	MG	2A	3204	1/1	0.97	0.20	50,50,50,50	0
56	MG	2A	3307	1/1	0.97	0.17	31,31,31,31	0
56	MG	1A	3451	1/1	0.97	0.20	20,20,20,20	0
56	MG	1A	3247	1/1	0.97	0.19	46,46,46,46	0
56	MG	1A	3186	1/1	0.97	0.12	53,53,53,53	0
56	MG	1a	1646	1/1	0.97	0.20	42,42,42,42	0
56	MG	2a	3078	1/1	0.97	0.20	71,71,71,71	0
56	MG	2A	3060	1/1	0.97	0.17	62,62,62,62	0
56	MG	1A	3356	1/1	0.97	0.45	45,45,45,45	0
56	MG	1A	3432	1/1	0.97	0.21	40,40,40,40	0
56	MG	1A	3445	1/1	0.97	0.22	46,46,46,46	0
56	MG	2A	3487	1/1	0.97	0.20	59,59,59,59	0
56	MG	1A	3195	1/1	0.97	0.13	32,32,32,32	0
56	MG	1A	3021	1/1	0.97	0.22	37,37,37,37	0
56	MG	1e	201	1/1	0.97	0.07	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3528	1/1	0.97	0.09	43,43,43,43	0
56	MG	1A	3815	1/1	0.97	0.16	30,30,30,30	0
56	MG	1A	3392	1/1	0.97	0.17	23,23,23,23	0
56	MG	2A	3477	1/1	0.97	0.13	28,28,28,28	0
56	MG	1A	3379	1/1	0.97	0.15	38,38,38,38	0
56	MG	1A	3482	1/1	0.97	0.17	37,37,37,37	0
56	MG	1A	3417	1/1	0.97	0.09	30,30,30,30	0
56	MG	1A	3030	1/1	0.97	0.91	32,32,32,32	0
56	MG	1A	3569	1/1	0.97	0.21	43,43,43,43	0
56	MG	2q	202	1/1	0.97	0.20	77,77,77,77	0
56	MG	1A	3630	1/1	0.97	0.24	33,33,33,33	0
56	MG	1A	3708	1/1	0.97	0.13	49,49,49,49	0
56	MG	1a	1633	1/1	0.97	0.14	56,56,56,56	0
56	MG	2A	3268	1/1	0.97	0.14	19,19,19,19	0
56	MG	1A	3157	1/1	0.97	0.12	46,46,46,46	0
56	MG	2a	3107	1/1	0.97	0.28	36,36,36,36	0
56	MG	1A	3060	1/1	0.97	0.14	40,40,40,40	0
57	ZN	1n	103	1/1	0.97	0.12	72,72,72,72	0
56	MG	1A	3814	1/1	0.97	0.14	39,39,39,39	0
56	MG	2A	3222	1/1	0.97	0.10	47,47,47,47	0
56	MG	2A	3426	1/1	0.97	0.36	45,45,45,45	0
56	MG	1A	3258	1/1	0.97	0.16	26,26,26,26	0
56	MG	2A	3425	1/1	0.97	0.23	41,41,41,41	0
56	MG	1A	3101	1/1	0.97	0.32	36,36,36,36	0
56	MG	10	105	1/1	0.97	0.26	35,35,35,35	0
56	MG	1A	3372	1/1	0.97	0.17	34,34,34,34	0
56	MG	2A	3258	1/1	0.97	0.08	32,32,32,32	0
56	MG	1A	3636	1/1	0.97	0.07	29,29,29,29	0
56	MG	1A	3105	1/1	0.97	0.72	35,35,35,35	0
56	MG	1A	3836	1/1	0.97	0.10	45,45,45,45	0
56	MG	1a	1624	1/1	0.97	0.10	60,60,60,60	0
56	MG	1A	3611	1/1	0.97	0.14	42,42,42,42	0
56	MG	1A	3461	1/1	0.97	0.23	52,52,52,52	0
56	MG	2A	3282	1/1	0.97	0.06	58,58,58,58	0
56	MG	2A	3400	1/1	0.97	0.13	38,38,38,38	0
56	MG	2a	3044	1/1	0.97	0.09	67,67,67,67	0
56	MG	1A	3539	1/1	0.97	0.13	32,32,32,32	0
56	MG	2A	3169	1/1	0.97	0.27	42,42,42,42	0
56	MG	12	102	1/1	0.97	0.57	50,50,50,50	0
56	MG	1A	3470	1/1	0.97	0.38	40,40,40,40	0
56	MG	1A	3517	1/1	0.97	0.11	43,43,43,43	0
56	MG	1B	206	1/1	0.97	0.15	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3632	1/1	0.97	0.08	36,36,36,36	0
56	MG	1A	3789	1/1	0.97	0.16	29,29,29,29	0
56	MG	1A	3427	1/1	0.97	0.18	39,39,39,39	0
56	MG	2A	3049	1/1	0.97	0.16	41,41,41,41	0
56	MG	1A	3634	1/1	0.97	0.13	40,40,40,40	0
56	MG	2A	3301	1/1	0.97	0.23	47,47,47,47	0
56	MG	2A	3593	1/1	0.97	0.12	45,45,45,45	0
56	MG	1B	209	1/1	0.97	0.18	48,48,48,48	0
56	MG	2A	3098	1/1	0.97	0.14	35,35,35,35	0
56	MG	1E	308	1/1	0.97	0.18	39,39,39,39	0
56	MG	1A	3671	1/1	0.97	0.15	41,41,41,41	0
56	MG	1A	3564	1/1	0.97	0.13	20,20,20,20	0
56	MG	1P	203	1/1	0.97	0.53	25,25,25,25	0
56	MG	1a	1712	1/1	0.97	0.27	40,40,40,40	0
56	MG	1A	3096	1/1	0.97	0.29	41,41,41,41	0
56	MG	1a	1670	1/1	0.97	0.17	34,34,34,34	0
56	MG	2A	3549	1/1	0.97	0.08	57,57,57,57	0
56	MG	1A	3766	1/1	0.97	0.08	57,57,57,57	0
56	MG	1A	3188	1/1	0.97	0.40	29,29,29,29	0
56	MG	1a	1731	1/1	0.97	0.21	34,34,34,34	0
56	MG	2A	3032	1/1	0.97	0.23	33,33,33,33	0
56	MG	1A	3846	1/1	0.97	0.14	30,30,30,30	0
56	MG	1A	3678	1/1	0.97	0.07	35,35,35,35	0
56	MG	1A	3653	1/1	0.97	0.49	43,43,43,43	0
56	MG	2A	3043	1/1	0.97	0.10	44,44,44,44	0
56	MG	1A	3726	1/1	0.97	0.14	36,36,36,36	0
56	MG	2A	3526	1/1	0.97	0.13	61,61,61,61	0
56	MG	1a	1602	1/1	0.97	0.14	51,51,51,51	0
56	MG	17	3102	1/1	0.97	0.21	27,27,27,27	0
56	MG	2A	3555	1/1	0.97	0.15	37,37,37,37	0
56	MG	2A	3358	1/1	0.97	0.16	43,43,43,43	0
56	MG	1A	3519	1/1	0.97	0.09	31,31,31,31	0
56	MG	2A	3466	1/1	0.97	0.10	56,56,56,56	0
56	MG	1A	3263	1/1	0.97	0.75	38,38,38,38	0
56	MG	1A	3351	1/1	0.97	0.12	49,49,49,49	0
56	MG	1A	3494	1/1	0.97	0.08	24,24,24,24	0
56	MG	2A	3057	1/1	0.97	0.07	44,44,44,44	0
56	MG	1A	3504	1/1	0.97	0.12	49,49,49,49	0
56	MG	2A	3214	1/1	0.97	0.33	36,36,36,36	0
56	MG	2a	3099	1/1	0.97	0.23	45,45,45,45	0
56	MG	1a	1629	1/1	0.97	0.17	58,58,58,58	0
56	MG	2A	3499	1/1	0.97	0.11	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3342	1/1	0.97	0.23	53,53,53,53	0
56	MG	1A	3596	1/1	0.97	0.14	40,40,40,40	0
56	MG	1A	3402	1/1	0.97	0.21	46,46,46,46	0
56	MG	1A	3842	1/1	0.97	0.15	42,42,42,42	0
56	MG	1A	3205	1/1	0.97	0.26	27,27,27,27	0
56	MG	1A	3521	1/1	0.97	0.07	22,22,22,22	0
56	MG	1A	3070	1/1	0.97	0.11	32,32,32,32	0
56	MG	2A	3618	1/1	0.97	0.28	54,54,54,54	0
56	MG	2A	3203	1/1	0.97	0.14	45,45,45,45	0
56	MG	1A	3714	1/1	0.97	0.20	51,51,51,51	0
56	MG	2A	3559	1/1	0.97	0.11	64,64,64,64	0
56	MG	2A	3360	1/1	0.97	0.14	32,32,32,32	0
56	MG	1A	3208	1/1	0.97	0.16	41,41,41,41	0
56	MG	1A	3707	1/1	0.97	0.26	48,48,48,48	0
56	MG	2A	3238	1/1	0.97	0.44	45,45,45,45	0
56	MG	1A	3153	1/1	0.97	0.16	33,33,33,33	0
56	MG	1a	1661	1/1	0.97	0.23	45,45,45,45	0
56	MG	1A	3556	1/1	0.97	0.13	48,48,48,48	0
56	MG	1A	3368	1/1	0.97	0.09	51,51,51,51	0
56	MG	1A	3370	1/1	0.97	0.25	39,39,39,39	0
56	MG	1a	1714	1/1	0.97	0.15	32,32,32,32	0
56	MG	1A	3080	1/1	0.97	0.25	45,45,45,45	0
56	MG	2A	3552	1/1	0.97	0.08	60,60,60,60	0
56	MG	2A	3182	1/1	0.97	0.44	58,58,58,58	0
56	MG	1a	1708	1/1	0.97	0.26	42,42,42,42	0
56	MG	1a	1691	1/1	0.97	0.19	42,42,42,42	0
56	MG	1A	3391	1/1	0.97	0.76	35,35,35,35	0
56	MG	1A	3833	1/1	0.97	0.23	56,56,56,56	0
56	MG	1A	3758	1/1	0.98	0.07	26,26,26,26	0
56	MG	2A	3602	1/1	0.98	0.18	55,55,55,55	0
56	MG	1A	3438	1/1	0.98	0.16	60,60,60,60	0
56	MG	1A	3018	1/1	0.98	0.10	48,48,48,48	0
57	ZN	29	501	1/1	0.98	0.12	67,67,67,67	0
56	MG	1A	3779	1/1	0.98	0.11	33,33,33,33	0
56	MG	2A	3007	1/1	0.98	0.13	49,49,49,49	0
56	MG	1A	3087	1/1	0.98	0.11	23,23,23,23	0
56	MG	1A	3376	1/1	0.98	0.19	25,25,25,25	0
56	MG	2A	3064	1/1	0.98	0.11	37,37,37,37	0
56	MG	1A	3584	1/1	0.98	0.08	40,40,40,40	0
56	MG	2A	3476	1/1	0.98	0.16	48,48,48,48	0
56	MG	1A	3100	1/1	0.98	0.56	51,51,51,51	0
56	MG	2A	3038	1/1	0.98	0.12	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3592	1/1	0.98	0.08	38,38,38,38	0
56	MG	1A	3075	1/1	0.98	0.14	28,28,28,28	0
56	MG	1A	3098	1/1	0.98	0.21	54,54,54,54	0
56	MG	1A	3641	1/1	0.98	0.17	23,23,23,23	0
56	MG	2A	3103	1/1	0.98	0.18	57,57,57,57	0
56	MG	1A	3114	1/1	0.98	0.54	37,37,37,37	0
56	MG	1A	3281	1/1	0.98	0.16	45,45,45,45	0
56	MG	1A	3481	1/1	0.98	0.11	31,31,31,31	0
56	MG	1A	3135	1/1	0.98	0.45	38,38,38,38	0
56	MG	2A	3556	1/1	0.98	0.07	68,68,68,68	0
56	MG	1A	3136	1/1	0.98	0.14	32,32,32,32	0
56	MG	1A	3656	1/1	0.98	0.05	52,52,52,52	0
56	MG	1a	1620	1/1	0.98	0.08	55,55,55,55	0
56	MG	2A	3379	1/1	0.98	0.18	34,34,34,34	0
56	MG	1A	3123	1/1	0.98	0.09	23,23,23,23	0
56	MG	1A	3619	1/1	0.98	0.11	39,39,39,39	0
56	MG	2A	3140	1/1	0.98	0.31	34,34,34,34	0
56	MG	2A	3327	1/1	0.98	0.18	40,40,40,40	0
56	MG	1A	3583	1/1	0.98	0.10	63,63,63,63	0
56	MG	1A	3367	1/1	0.98	0.34	41,41,41,41	0
56	MG	2A	3415	1/1	0.98	0.16	35,35,35,35	0
56	MG	2A	3279	1/1	0.98	0.23	27,27,27,27	0
56	MG	1A	3791	1/1	0.98	0.09	41,41,41,41	0
56	MG	1A	3031	1/1	0.98	0.24	43,43,43,43	0
56	MG	2A	3022	1/1	0.98	0.14	43,43,43,43	0
56	MG	1A	3535	1/1	0.98	0.11	20,20,20,20	0
56	MG	1A	3215	1/1	0.98	0.27	49,49,49,49	0
56	MG	2A	3288	1/1	0.98	0.14	38,38,38,38	0
56	MG	1a	1715	1/1	0.98	0.15	42,42,42,42	0
56	MG	1A	3637	1/1	0.98	0.15	58,58,58,58	0
56	MG	1A	3056	1/1	0.98	0.19	33,33,33,33	0
56	MG	1A	3088	1/1	0.98	0.70	41,41,41,41	0
56	MG	1A	3468	1/1	0.98	0.09	29,29,29,29	0
56	MG	1A	3544	1/1	0.98	0.12	30,30,30,30	0
56	MG	2A	3159	1/1	0.98	0.12	44,44,44,44	0
56	MG	2A	3509	1/1	0.98	0.07	57,57,57,57	0
56	MG	1A	3418	1/1	0.98	0.16	28,28,28,28	0
56	MG	1A	3771	1/1	0.98	0.20	37,37,37,37	0
56	MG	1A	3462	1/1	0.98	0.10	32,32,32,32	0
56	MG	1A	3292	1/1	0.98	0.17	33,33,33,33	0
56	MG	18	104	1/1	0.98	0.18	18,18,18,18	0
56	MG	1A	3004	1/1	0.98	0.53	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3185	1/1	0.98	0.48	34,34,34,34	0
56	MG	1A	3178	1/1	0.98	0.11	54,54,54,54	0
56	MG	18	102	1/1	0.98	0.21	42,42,42,42	0
56	MG	2A	3084	1/1	0.98	0.11	68,68,68,68	0
56	MG	2A	3093	1/1	0.98	0.16	30,30,30,30	0
56	MG	2A	3580	1/1	0.98	0.09	31,31,31,31	0
56	MG	1a	1733	1/1	0.98	0.25	25,25,25,25	0
56	MG	1D	307	1/1	0.98	0.23	46,46,46,46	0
56	MG	1A	3086	1/1	0.98	0.41	33,33,33,33	0
56	MG	1A	3790	1/1	0.98	0.12	34,34,34,34	0
56	MG	2a	3043	1/1	0.98	0.23	64,64,64,64	0
56	MG	1A	3025	1/1	0.98	0.54	48,48,48,48	0
56	MG	1A	3147	1/1	0.98	0.40	48,48,48,48	0
56	MG	1A	3571	1/1	0.98	0.11	29,29,29,29	0
56	MG	1A	3685	1/1	0.98	0.10	56,56,56,56	0
56	MG	21	101	1/1	0.98	0.41	62,62,62,62	0
56	MG	1A	3191	1/1	0.98	0.51	41,41,41,41	0
56	MG	1B	202	1/1	0.98	0.22	30,30,30,30	0
56	MG	1A	3580	1/1	0.98	0.12	39,39,39,39	0
56	MG	2A	3342	1/1	0.98	0.21	21,21,21,21	0
56	MG	1a	1736	1/1	0.98	0.07	27,27,27,27	0
56	MG	1A	3006	1/1	0.98	0.23	36,36,36,36	0
56	MG	1A	3628	1/1	0.98	0.07	68,68,68,68	0
56	MG	1A	3577	1/1	0.98	0.09	61,61,61,61	0
56	MG	1A	3606	1/1	0.98	0.25	32,32,32,32	0
56	MG	1A	3834	1/1	0.98	0.13	39,39,39,39	0
56	MG	1A	3016	1/1	0.98	0.22	32,32,32,32	0
56	MG	2A	3066	1/1	0.98	0.17	51,51,51,51	0
56	MG	1l	201	1/1	0.98	0.10	56,56,56,56	0
56	MG	1A	3705	1/1	0.98	0.09	45,45,45,45	0
56	MG	2A	3582	1/1	0.98	0.23	49,49,49,49	0
56	MG	2A	3181	1/1	0.98	0.15	57,57,57,57	0
56	MG	1A	3064	1/1	0.98	0.19	58,58,58,58	0
56	MG	2A	3058	1/1	0.98	0.19	30,30,30,30	0
56	MG	1A	3331	1/1	0.98	0.32	56,56,56,56	0
56	MG	2A	3176	1/1	0.98	0.41	56,56,56,56	0
56	MG	1B	207	1/1	0.98	0.14	44,44,44,44	0
56	MG	2a	3088	1/1	0.98	0.21	48,48,48,48	0
56	MG	1D	302	1/1	0.98	0.24	32,32,32,32	0
56	MG	2A	3468	1/1	0.98	0.13	29,29,29,29	0
56	MG	2A	3603	1/1	0.98	0.20	61,61,61,61	0
56	MG	1A	3652	1/1	0.98	0.09	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	ZN	26	102	1/1	0.98	0.20	64,64,64,64	0
56	MG	2A	3410	1/1	0.98	0.27	32,32,32,32	0
56	MG	1A	3810	1/1	0.98	0.16	25,25,25,25	0
56	MG	1A	3282	1/1	0.98	0.10	40,40,40,40	0
56	MG	1A	3363	1/1	0.98	0.15	28,28,28,28	0
56	MG	2A	3473	1/1	0.98	0.15	35,35,35,35	0
56	MG	1A	3211	1/1	0.98	0.11	38,38,38,38	0
56	MG	1A	3566	1/1	0.98	0.17	38,38,38,38	0
56	MG	2q	201	1/1	0.98	0.16	54,54,54,54	0
56	MG	1a	1699	1/1	0.98	0.21	27,27,27,27	0
56	MG	1A	3518	1/1	0.98	0.23	27,27,27,27	0
56	MG	1a	1614	1/1	0.98	0.11	52,52,52,52	0
56	MG	1A	3472	1/1	0.98	0.13	27,27,27,27	0
56	MG	1A	3378	1/1	0.98	0.48	29,29,29,29	0
56	MG	1A	3238	1/1	0.98	0.20	43,43,43,43	0
56	MG	1A	3659	1/1	0.98	0.15	56,56,56,56	0
56	MG	1A	3062	1/1	0.98	0.16	28,28,28,28	0
56	MG	2A	3345	1/1	0.98	0.22	56,56,56,56	0
56	MG	1A	3699	1/1	0.98	0.10	61,61,61,61	0
56	MG	1A	3118	1/1	0.98	0.40	38,38,38,38	0
56	MG	1A	3162	1/1	0.98	0.34	36,36,36,36	0
56	MG	2A	3099	1/1	0.98	0.21	44,44,44,44	0
56	MG	1A	3277	1/1	0.98	0.07	61,61,61,61	0
56	MG	1A	3800	1/1	0.98	0.09	30,30,30,30	0
56	MG	2A	3510	1/1	0.98	0.16	56,56,56,56	0
56	MG	1a	1665	1/1	0.98	0.22	40,40,40,40	0
56	MG	1A	3684	1/1	0.98	0.11	30,30,30,30	0
56	MG	2A	3594	1/1	0.98	0.22	42,42,42,42	0
56	MG	1T	202	1/1	0.98	0.36	43,43,43,43	0
56	MG	2A	3583	1/1	0.98	0.25	63,63,63,63	0
56	MG	1A	3415	1/1	0.98	0.17	36,36,36,36	0
56	MG	1a	1766	1/1	0.98	0.30	32,32,32,32	0
56	MG	1A	3579	1/1	0.98	0.07	41,41,41,41	0
56	MG	1A	3164	1/1	0.98	0.13	49,49,49,49	0
56	MG	1a	1743	1/1	0.98	0.26	34,34,34,34	0
56	MG	1A	3111	1/1	0.98	0.09	42,42,42,42	0
58	SF4	2d	302	8/8	0.98	0.14	71,76,86,97	0
56	MG	1A	3742	1/1	0.98	0.16	29,29,29,29	0
56	MG	1A	3839	1/1	0.98	0.14	46,46,46,46	0
56	MG	2A	3218	1/1	0.98	0.23	49,49,49,49	0
56	MG	1A	3374	1/1	0.98	0.17	43,43,43,43	0
56	MG	2A	3611	1/1	0.98	0.16	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1m	3001	1/1	0.98	0.15	51,51,51,51	0
56	MG	1A	3524	1/1	0.98	0.05	51,51,51,51	0
56	MG	2A	3008	1/1	0.98	0.15	47,47,47,47	0
56	MG	2A	3145	1/1	0.98	0.46	44,44,44,44	0
56	MG	1A	3058	1/1	0.98	0.17	29,29,29,29	0
56	MG	2A	3547	1/1	0.98	0.09	56,56,56,56	0
56	MG	2A	3239	1/1	0.98	0.04	56,56,56,56	0
56	MG	1A	3757	1/1	0.98	0.11	24,24,24,24	0
56	MG	1A	3554	1/1	0.98	0.12	25,25,25,25	0
56	MG	1a	1711	1/1	0.98	0.25	48,48,48,48	0
56	MG	1a	1668	1/1	0.98	0.16	31,31,31,31	0
56	MG	1F	309	1/1	0.98	0.09	40,40,40,40	0
56	MG	1A	3045	1/1	0.98	0.13	46,46,46,46	0
56	MG	1A	3713	1/1	0.98	0.80	51,51,51,51	0
56	MG	1A	3132	1/1	0.98	0.26	40,40,40,40	0
56	MG	1A	3283	1/1	0.98	0.33	53,53,53,53	0
56	MG	1A	3664	1/1	0.98	0.13	58,58,58,58	0
56	MG	1A	3492	1/1	0.98	0.20	50,50,50,50	0
57	ZN	25	103	1/1	0.98	0.16	51,51,51,51	0
56	MG	1A	3020	1/1	0.99	0.20	19,19,19,19	0
56	MG	2A	3015	1/1	0.99	0.37	39,39,39,39	0
56	MG	15	101	1/1	0.99	0.25	46,46,46,46	0
56	MG	2A	3154	1/1	0.99	0.11	31,31,31,31	0
56	MG	2A	3079	1/1	0.99	0.17	53,53,53,53	0
56	MG	1a	1720	1/1	0.99	0.14	54,54,54,54	0
56	MG	1A	3513	1/1	0.99	0.13	26,26,26,26	0
56	MG	2A	3348	1/1	0.99	0.22	30,30,30,30	0
56	MG	2A	3422	1/1	0.99	0.18	34,34,34,34	0
56	MG	2A	3458	1/1	0.99	0.13	42,42,42,42	0
56	MG	1A	3675	1/1	0.99	0.14	59,59,59,59	0
56	MG	1A	3035	1/1	0.99	0.10	33,33,33,33	0
56	MG	1A	3419	1/1	0.99	0.23	18,18,18,18	0
56	MG	1S	201	1/1	0.99	0.20	58,58,58,58	0
56	MG	1A	3698	1/1	0.99	0.16	34,34,34,34	0
56	MG	1A	3108	1/1	0.99	0.55	50,50,50,50	0
56	MG	1A	3397	1/1	0.99	0.12	25,25,25,25	0
56	MG	1A	3306	1/1	0.99	0.25	48,48,48,48	0
56	MG	1a	1664	1/1	0.99	0.10	31,31,31,31	0
56	MG	2P	201	1/1	0.99	0.24	47,47,47,47	0
56	MG	2A	3588	1/1	0.99	0.12	47,47,47,47	0
56	MG	1A	3068	1/1	0.99	0.15	24,24,24,24	0
56	MG	2V	201	1/1	0.99	0.45	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3441	1/1	0.99	0.31	21,21,21,21	0
56	MG	1A	3484	1/1	0.99	0.04	51,51,51,51	0
56	MG	2A	3461	1/1	0.99	0.15	46,46,46,46	0
56	MG	2A	3233	1/1	0.99	0.15	45,45,45,45	0
56	MG	1A	3515	1/1	0.99	0.10	30,30,30,30	0
56	MG	1A	3190	1/1	0.99	0.24	37,37,37,37	0
57	ZN	1Y	202	1/1	0.99	0.18	57,57,57,57	0
56	MG	2A	3092	1/1	0.99	0.12	49,49,49,49	0
56	MG	2A	3035	1/1	0.99	0.41	37,37,37,37	0
56	MG	1A	3139	1/1	0.99	0.33	32,32,32,32	0
56	MG	1A	3509	1/1	0.99	0.13	45,45,45,45	0
56	MG	1A	3441	1/1	0.99	0.09	32,32,32,32	0
56	MG	2a	3101	1/1	0.99	0.18	27,27,27,27	0
56	MG	2A	3306	1/1	0.99	0.12	35,35,35,35	0
56	MG	1A	3718	1/1	0.99	0.10	17,17,17,17	0
56	MG	2A	3286	1/1	0.99	0.29	29,29,29,29	0
56	MG	1A	3762	1/1	0.99	0.06	54,54,54,54	0
56	MG	1A	3489	1/1	0.99	0.13	19,19,19,19	0
56	MG	2A	3617	1/1	0.99	0.07	41,41,41,41	0
56	MG	1a	1738	1/1	0.99	0.27	46,46,46,46	0
56	MG	2A	3220	1/1	0.99	0.26	33,33,33,33	0
56	MG	2A	3616	1/1	0.99	0.23	25,25,25,25	0
56	MG	2A	3529	1/1	0.99	0.19	41,41,41,41	0
56	MG	2A	3257	1/1	0.99	0.59	51,51,51,51	0
56	MG	1A	3546	1/1	0.99	0.14	12,12,12,12	0
56	MG	1A	3109	1/1	0.99	0.11	33,33,33,33	0
56	MG	1A	3511	1/1	0.99	0.18	36,36,36,36	0
56	MG	1A	3782	1/1	0.99	0.11	39,39,39,39	0
56	MG	1D	304	1/1	0.99	0.30	35,35,35,35	0
56	MG	1A	3578	1/1	0.99	0.09	33,33,33,33	0
58	SF4	1d	302	8/8	0.99	0.17	57,68,71,74	0
56	MG	1P	202	1/1	0.99	0.59	31,31,31,31	0
56	MG	1a	1636	1/1	0.99	0.08	48,48,48,48	0
56	MG	1A	3192	1/1	0.99	0.21	44,44,44,44	0
56	MG	1D	301	1/1	0.99	0.37	37,37,37,37	0
56	MG	1A	3416	1/1	0.99	0.24	19,19,19,19	0
56	MG	1A	3560	1/1	0.99	0.11	33,33,33,33	0
56	MG	1A	3255	1/1	0.99	0.27	41,41,41,41	0
56	MG	2A	3018	1/1	0.99	0.11	44,44,44,44	0
57	ZN	16	501	1/1	0.99	0.18	45,45,45,45	0
56	MG	1A	3322	1/1	0.99	0.31	38,38,38,38	0
56	MG	1A	3023	1/1	0.99	0.31	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1B	216	1/1	0.99	0.07	46,46,46,46	0
56	MG	1A	3264	1/1	0.99	0.18	47,47,47,47	0
56	MG	1A	3508	1/1	0.99	0.16	26,26,26,26	0
56	MG	2A	3497	1/1	0.99	0.10	45,45,45,45	0
56	MG	1A	3194	1/1	0.99	0.15	52,52,52,52	0
56	MG	2A	3531	1/1	0.99	0.14	31,31,31,31	0
56	MG	1A	3065	1/1	0.99	0.14	33,33,33,33	0
56	MG	1A	3483	1/1	0.99	0.14	49,49,49,49	0
56	MG	1A	3003	1/1	0.99	0.16	29,29,29,29	0
57	ZN	15	106	1/1	0.99	0.17	44,44,44,44	0
57	ZN	19	102	1/1	1.00	0.16	42,42,42,42	0
56	MG	2A	3017	1/1	1.00	0.39	45,45,45,45	0
56	MG	1A	3261	1/1	1.00	0.13	38,38,38,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.