



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2022 – 09:23 PM EDT

PDB ID : 5DOY
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with antibiotic Hygromycin A, mRNA and three tRNAs in the A, P and E sites at 2.6Å resolution
Authors : Polikanov, Y.S.; Starosta, A.L.; Juette, M.F.; Altman, R.B.; Terry, D.S.; Lu, W.; Burnett, B.J.; Dinos, G.; Reynolds, K.; Blanchard, S.C.; Steitz, T.A.; Wilson, D.N.
Deposited on : 2015-09-11
Resolution : 2.60 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	:	2.28.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28.1

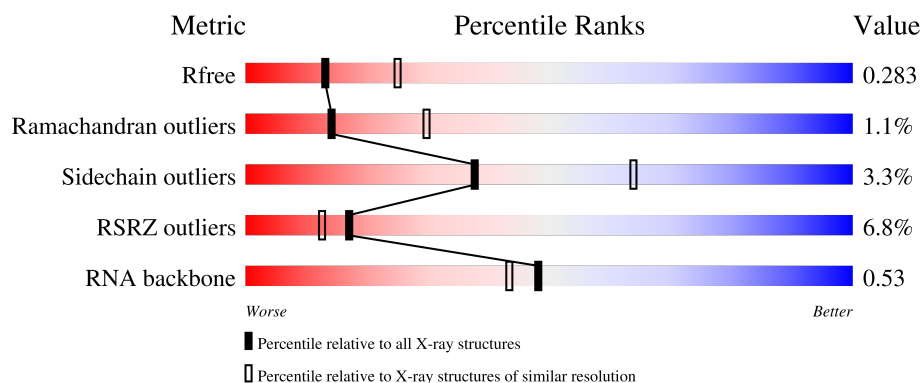
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)
RNA backbone	3102	1040 (2.90-2.30)

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

Mol	Chain	Length	Quality of chain
1	1A	2915	<div> <div>2%</div> <div>82%</div> <div>16%</div> <div>..</div> </div>
1	2A	2915	<div> <div>2%</div> <div>77%</div> <div>18%</div> <div>..</div> </div>
2	1B	121	<div> <div>92%</div> <div>7%</div> <div>..</div> </div>
2	2B	121	<div> <div>2%</div> <div>68%</div> <div>31%</div> <div>.</div> </div>
3	1D	276	<div> <div>4%</div> <div>97%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
3	2D	276	<div> <div>3%</div> <div>97%</div> <div>.</div> </div>
4	1E	206	<div> <div>%</div> <div>94%</div> <div>5%</div> <div>.</div> </div>
4	2E	206	<div> <div>2%</div> <div>92%</div> <div>7%</div> <div>.</div> </div>
5	1F	210	<div> <div>%</div> <div>91%</div> <div>6%</div> <div>.</div> </div>
5	2F	210	<div> <div>3%</div> <div>91%</div> <div>6%</div> <div>.</div> </div>
6	1G	182	<div> <div>5%</div> <div>94%</div> <div>5%</div> <div>.</div> </div>
6	2G	182	<div> <div>19%</div> <div>94%</div> <div>5%</div> <div>.</div> </div>
7	1H	180	<div> <div>2%</div> <div>94%</div> <div>.</div> <div>.</div> </div>
7	2H	180	<div> <div>14%</div> <div>94%</div> <div>.</div> <div>.</div> </div>
8	1I	148	<div> <div>%</div> <div>93%</div> <div>5%</div> <div>.</div> </div>
8	2I	148	<div> <div>%</div> <div>95%</div> <div>.</div> <div>.</div> </div>
9	1N	140	<div> <div>97%</div> <div>.</div> </div>
9	2N	140	<div> <div>21%</div> <div>98%</div> <div>.</div> </div>
10	1O	122	<div> <div>3%</div> <div>98%</div> <div>.</div> </div>
10	2O	122	<div> <div>12%</div> <div>99%</div> <div>.</div> </div>
11	1P	150	<div> <div>3%</div> <div>95%</div> <div>.</div> <div>.</div> </div>
11	2P	150	<div> <div>3%</div> <div>97%</div> <div>.</div> <div>.</div> </div>
12	1Q	141	<div> <div>6%</div> <div>99%</div> <div>.</div> </div>
12	2Q	141	<div> <div>37%</div> <div>98%</div> <div>.</div> </div>
13	1R	118	<div> <div>3%</div> <div>91%</div> <div>9%</div> </div>
13	2R	118	<div> <div>%</div> <div>92%</div> <div>8%</div> </div>
14	1S	112	<div> <div>%</div> <div>96%</div> <div>.</div> <div>.</div> </div>
14	2S	112	<div> <div>8%</div> <div>95%</div> <div>.</div> <div>.</div> </div>
15	1T	146	<div> <div>%</div> <div>88%</div> <div>.</div> <div>10%</div> </div>
15	2T	146	<div> <div>%</div> <div>89%</div> <div>.</div> <div>10%</div> </div>

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

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Mol	Chain	Length	Quality of chain
28	26	54	<div> <div>11%</div> <div>93%</div> <div>6%</div> </div>
29	17	49	<div> <div>8%</div> <div>96%</div> <div></div> </div>
29	27	49	<div> <div>8%</div> <div>94%</div> <div></div> </div>
30	18	65	<div> <div></div> <div>95%</div> <div></div> </div>
30	28	65	<div> <div></div> <div>95%</div> <div></div> </div>
31	19	37	<div> <div>11%</div> <div>100%</div> <div></div> </div>
31	29	37	<div> <div>30%</div> <div>95%</div> <div>5%</div> </div>
32	1a	1521	<div> <div>%</div> <div>82%</div> <div>16%</div> </div>
32	2a	1521	<div> <div>%</div> <div>82%</div> <div>17%</div> </div>
33	1b	256	<div> <div></div> <div>86%</div> <div>10%</div> </div>
33	2b	256	<div> <div>12%</div> <div>85%</div> <div>5%</div> </div>
34	1c	239	<div> <div>9%</div> <div>84%</div> <div>14%</div> </div>
34	2c	239	<div> <div>28%</div> <div>85%</div> <div>14%</div> </div>
35	1d	209	<div> <div>14%</div> <div>97%</div> <div></div> </div>
35	2d	209	<div> <div>30%</div> <div>98%</div> <div></div> </div>
36	1e	162	<div> <div>5%</div> <div>88%</div> <div>9%</div> </div>
36	2e	162	<div> <div>23%</div> <div>90%</div> <div>9%</div> </div>
37	1f	101	<div> <div>8%</div> <div>99%</div> <div></div> </div>
37	2f	101	<div> <div>%</div> <div>99%</div> <div></div> </div>
38	1g	156	<div> <div>12%</div> <div>98%</div> <div></div> </div>
38	2g	156	<div> <div>12%</div> <div>96%</div> <div></div> </div>
39	1h	138	<div> <div>4%</div> <div>98%</div> <div></div> </div>
39	2h	138	<div> <div>19%</div> <div>98%</div> <div></div> </div>
40	1i	128	<div> <div>6%</div> <div>96%</div> <div></div> </div>
40	2i	128	<div> <div>23%</div> <div>95%</div> <div></div> </div>

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

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Mol	Chain	Length	Quality of chain
53	2v	27	
54	1w	76	
54	1y	76	
54	2w	76	
54	2y	76	
55	1x	77	
55	2x	77	

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	3722	-	-	-	X
56	MG	1A	3770	-	-	-	X
56	MG	1A	3847	-	-	-	X
56	MG	2A	3197	-	-	-	X
56	MG	2O	8002	-	-	-	X

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 298925 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
			1429	916	256	253	4			
6	2G	181	Total	C	N	O	S	0	0	0
			1428	913	258	253	4			

- Molecule 7 is a protein called 50S Ribosomal Protein L6.

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

- Molecule 8 is a protein called 50S Ribosomal Protein L9.

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

- Molecule 9 is a protein called 50S Ribosomal Protein L13.

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

- Molecule 10 is a protein called 50S Ribosomal Protein L14.

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

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

- Molecule 11 is a protein called 50S Ribosomal Protein L15.

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

- Molecule 12 is a protein called 50S Ribosomal Protein L16.

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

- Molecule 13 is a protein called 50S Ribosomal Protein L17.

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

- Molecule 14 is a protein called 50S Ribosomal Protein L18.

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

- Molecule 15 is a protein called 50S Ribosomal Protein L19.

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

- Molecule 16 is a protein called 50S Ribosomal Protein L20.

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

- Molecule 17 is a protein called 50S Ribosomal Protein L21.

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

- Molecule 18 is a protein called 50S Ribosomal Protein L22.

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

- Molecule 19 is a protein called 50S Ribosomal Protein L23.

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

- Molecule 20 is a protein called 50S Ribosomal Protein L24.

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

- Molecule 21 is a protein called 50S Ribosomal Protein L25.

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

- Molecule 22 is a protein called 50S Ribosomal Protein L27.

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

- Molecule 23 is a protein called 50S Ribosomal Protein L28.

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

- Molecule 24 is a protein called 50S Ribosomal Protein L29.

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

- Molecule 25 is a protein called 50S Ribosomal Protein L30.

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

- Molecule 26 is a protein called 50S Ribosomal Protein L31.

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

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

- Molecule 27 is a protein called 50S Ribosomal Protein L32.

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

- Molecule 28 is a protein called 50S Ribosomal Protein L33.

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

- Molecule 29 is a protein called 50S Ribosomal Protein L34.

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

- Molecule 30 is a protein called 50S Ribosomal Protein L35.

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

- Molecule 31 is a protein called 50S Ribosomal Protein L36.

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

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

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

- Molecule 33 is a protein called 30S Ribosomal Protein S2.

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

- Molecule 34 is a protein called 30S Ribosomal Protein S3.

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

- Molecule 35 is a protein called 30S Ribosomal Protein S4.

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

- Molecule 36 is a protein called 30S Ribosomal Protein S5.

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

- Molecule 37 is a protein called 30S Ribosomal Protein S6.

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

- Molecule 38 is a protein called 30S Ribosomal Protein S7.

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

- Molecule 39 is a protein called 30S Ribosomal Protein S8.

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

- Molecule 40 is a protein called 30S Ribosomal Protein S9.

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

- Molecule 41 is a protein called 30S Ribosomal Protein S10.

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

- Molecule 42 is a protein called 30S Ribosomal Protein S11.

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

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

- Molecule 43 is a protein called 30S Ribosomal Protein S12.

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

- Molecule 44 is a protein called 30S Ribosomal Protein S13.

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

- Molecule 45 is a protein called 30S Ribosomal Protein S14.

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	14	Total	C	N	O	P	0	0	0
			281	125	51	91	14			
53	2v	13	Total	C	N	O	P	0	0	0
			277	125	51	88	13			

- Molecule 54 is a RNA chain called A-site and E-site tRNAs.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
54	1w	75	Total 1574	C 704	N 283	O 512	P 73	S 2	0	0	1
54	1y	74	Total 1581	C 707	N 285	O 515	P 73	S 1	0	0	0
54	2w	74	Total 1547	C 688	N 278	O 507	P 73	S 1	0	0	1
54	2y	73	Total 1561	C 698	N 283	O 507	P 72	S 1	0	0	0

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
55	1x	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			
55	2x	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1A	963	Total	Mg	0	0
			963	963		
56	1B	29	Total	Mg	0	0
			29	29		
56	1D	5	Total	Mg	0	0
			5	5		
56	1E	6	Total	Mg	0	0
			6	6		
56	1F	7	Total	Mg	0	0
			7	7		
56	1G	4	Total	Mg	0	0
			4	4		
56	1I	1	Total	Mg	0	0
			1	1		
56	1N	7	Total	Mg	0	0
			7	7		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1O	6	Total 6	Mg 6	0	0
56	1P	4	Total 4	Mg 4	0	0
56	1Q	6	Total 6	Mg 6	0	0
56	1R	3	Total 3	Mg 3	0	0
56	1S	2	Total 2	Mg 2	0	0
56	1T	3	Total 3	Mg 3	0	0
56	1U	5	Total 5	Mg 5	0	0
56	1V	2	Total 2	Mg 2	0	0
56	1W	6	Total 6	Mg 6	0	0
56	1X	4	Total 4	Mg 4	0	0
56	1Y	1	Total 1	Mg 1	0	0
56	1Z	5	Total 5	Mg 5	0	0
56	10	4	Total 4	Mg 4	0	0
56	11	3	Total 3	Mg 3	0	0
56	12	1	Total 1	Mg 1	0	0
56	13	3	Total 3	Mg 3	0	0
56	15	2	Total 2	Mg 2	0	0
56	16	1	Total 1	Mg 1	0	0
56	17	2	Total 2	Mg 2	0	0
56	18	2	Total 2	Mg 2	0	0
56	19	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1a	239	Total 239	Mg 239	0	0
56	1b	2	Total 2	Mg 2	0	0
56	1d	2	Total 2	Mg 2	0	0
56	1e	1	Total 1	Mg 1	0	0
56	1f	2	Total 2	Mg 2	0	0
56	1l	3	Total 3	Mg 3	0	0
56	1t	1	Total 1	Mg 1	0	0
56	1v	1	Total 1	Mg 1	0	0
56	1w	6	Total 6	Mg 6	0	0
56	1x	10	Total 10	Mg 10	0	0
56	1y	2	Total 2	Mg 2	0	0
56	2A	673	Total 673	Mg 673	0	0
56	2B	18	Total 18	Mg 18	0	0
56	2D	4	Total 4	Mg 4	0	0
56	2E	5	Total 5	Mg 5	0	0
56	2F	4	Total 4	Mg 4	0	0
56	2G	1	Total 1	Mg 1	0	0
56	2O	2	Total 2	Mg 2	0	0
56	2P	1	Total 1	Mg 1	0	0
56	2Q	4	Total 4	Mg 4	0	0
56	2R	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2T	1	Total 1	Mg 1	0	0
56	2U	4	Total 4	Mg 4	0	0
56	2V	1	Total 1	Mg 1	0	0
56	2X	1	Total 1	Mg 1	0	0
56	2Z	1	Total 1	Mg 1	0	0
56	20	3	Total 3	Mg 3	0	0
56	23	1	Total 1	Mg 1	0	0
56	26	1	Total 1	Mg 1	0	0
56	28	1	Total 1	Mg 1	0	0
56	2a	196	Total 196	Mg 196	0	0
56	2d	1	Total 1	Mg 1	0	0
56	2e	1	Total 1	Mg 1	0	0
56	2f	2	Total 2	Mg 2	0	0
56	2g	1	Total 1	Mg 1	0	0
56	2j	2	Total 2	Mg 2	0	0
56	2l	2	Total 2	Mg 2	0	0
56	2p	1	Total 1	Mg 1	0	0
56	2q	2	Total 2	Mg 2	0	0
56	2r	1	Total 1	Mg 1	0	0
56	2t	1	Total 1	Mg 1	0	0
56	2v	1	Total 1	Mg 1	0	0

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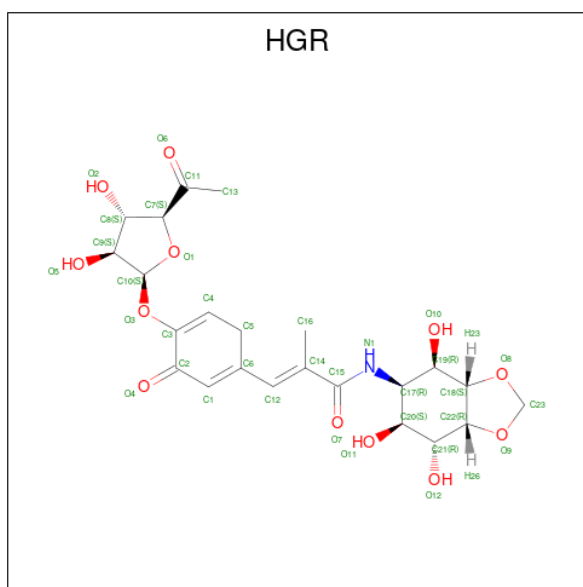
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2w	3	Total	Mg	0	0
			3	3		
56	2x	2	Total	Mg	0	0
			2	2		

- Molecule 57 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1A	1	Total	K	0	0
			1	1		
57	2A	1	Total	K	0	0
			1	1		

- Molecule 58 is Hygromycin A (three-letter code: HGR) (formula: C₂₃H₂₉NO₁₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
58	1A	1	Total	C	N	O	0	0
			36	23	1	12		
58	2A	1	Total	C	N	O	0	0
			36	23	1	12		

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

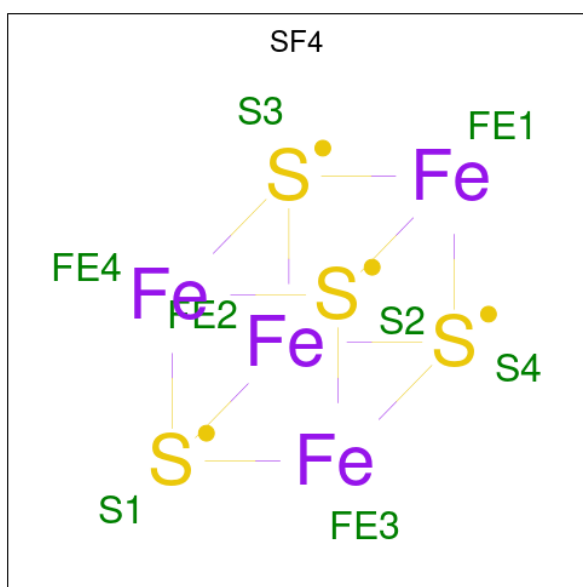
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1Y	1	Total	Zn	0	0
			1	1		

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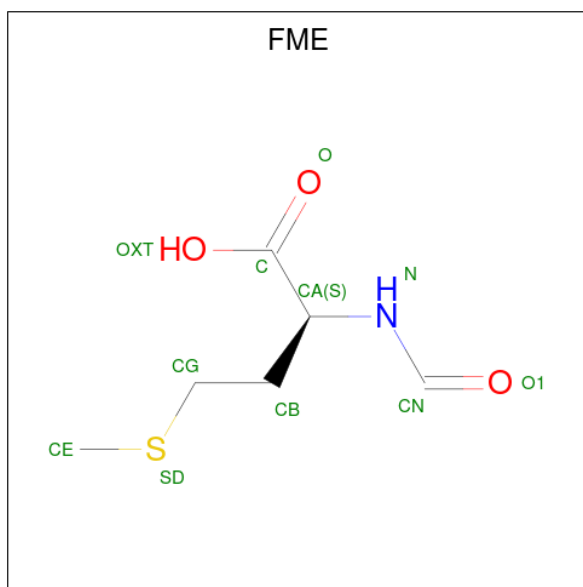
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	14	1	Total 1	Zn 1	0	0
59	15	1	Total 1	Zn 1	0	0
59	16	1	Total 1	Zn 1	0	0
59	19	1	Total 1	Zn 1	0	0
59	1n	1	Total 1	Zn 1	0	0
59	2Y	1	Total 1	Zn 1	0	0
59	24	1	Total 1	Zn 1	0	0
59	25	1	Total 1	Zn 1	0	0
59	26	1	Total 1	Zn 1	0	0
59	29	1	Total 1	Zn 1	0	0
59	2n	1	Total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

- Molecule 60 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

- Molecule 61 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: $C_6H_{11}NO_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
61	1x	1	Total	C	N	O	S	0	0
			10	6	1	2	1		
61	2x	1	Total	C	N	O	S	0	0
			10	6	1	2	1		

- Molecule 62 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	1A	1577	Total	O	0	0
			1577	1577		
62	1B	43	Total	O	0	0
			43	43		
62	1D	23	Total	O	0	0
			23	23		
62	1E	25	Total	O	0	0
			25	25		
62	1F	17	Total	O	0	0
			17	17		
62	1G	3	Total	O	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	1H	1	Total 1	O 1	0	0
62	1N	3	Total 3	O 3	0	0
62	1O	4	Total 4	O 4	0	0
62	1P	20	Total 20	O 20	0	0
62	1Q	4	Total 4	O 4	0	0
62	1R	5	Total 5	O 5	0	0
62	1S	3	Total 3	O 3	0	0
62	1T	4	Total 4	O 4	0	0
62	1U	9	Total 9	O 9	0	0
62	1V	5	Total 5	O 5	0	0
62	1W	8	Total 8	O 8	0	0
62	1X	7	Total 7	O 7	0	0
62	1Y	2	Total 2	O 2	0	0
62	1Z	1	Total 1	O 1	0	0
62	10	9	Total 9	O 9	0	0
62	11	3	Total 3	O 3	0	0
62	12	4	Total 4	O 4	0	0
62	13	3	Total 3	O 3	0	0
62	14	1	Total 1	O 1	0	0
62	15	4	Total 4	O 4	0	0
62	16	2	Total 2	O 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	17	5	Total O 5 5	0	0
62	18	10	Total O 10 10	0	0
62	19	1	Total O 1 1	0	0
62	1a	287	Total O 287 287	0	0
62	1e	1	Total O 1 1	0	0
62	1h	1	Total O 1 1	0	0
62	1i	1	Total O 1 1	0	0
62	1l	4	Total O 4 4	0	0
62	1m	1	Total O 1 1	0	0
62	1n	1	Total O 1 1	0	0
62	1o	1	Total O 1 1	0	0
62	1p	1	Total O 1 1	0	0
62	1q	1	Total O 1 1	0	0
62	1s	1	Total O 1 1	0	0
62	1v	3	Total O 3 3	0	0
62	1w	8	Total O 8 8	0	0
62	1x	6	Total O 6 6	0	0
62	1y	1	Total O 1 1	0	0
62	2A	1063	Total O 1063 1063	0	0
62	2B	10	Total O 10 10	0	0
62	2D	20	Total O 20 20	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	2E	9	Total	O	0	0
			9	9		
62	2F	7	Total	O	0	0
			7	7		
62	2I	1	Total	O	0	0
			1	1		
62	2N	2	Total	O	0	0
			2	2		
62	2O	1	Total	O	0	0
			1	1		
62	2P	14	Total	O	0	0
			14	14		
62	2Q	1	Total	O	0	0
			1	1		
62	2R	3	Total	O	0	0
			3	3		
62	2T	2	Total	O	0	0
			2	2		
62	2U	1	Total	O	0	0
			1	1		
62	2V	2	Total	O	0	0
			2	2		
62	2W	2	Total	O	0	0
			2	2		
62	2X	3	Total	O	0	0
			3	3		
62	2Y	1	Total	O	0	0
			1	1		
62	2Z	1	Total	O	0	0
			1	1		
62	20	4	Total	O	0	0
			4	4		
62	21	3	Total	O	0	0
			3	3		
62	23	1	Total	O	0	0
			1	1		
62	25	2	Total	O	0	0
			2	2		
62	26	2	Total	O	0	0
			2	2		
62	28	5	Total	O	0	0
			5	5		

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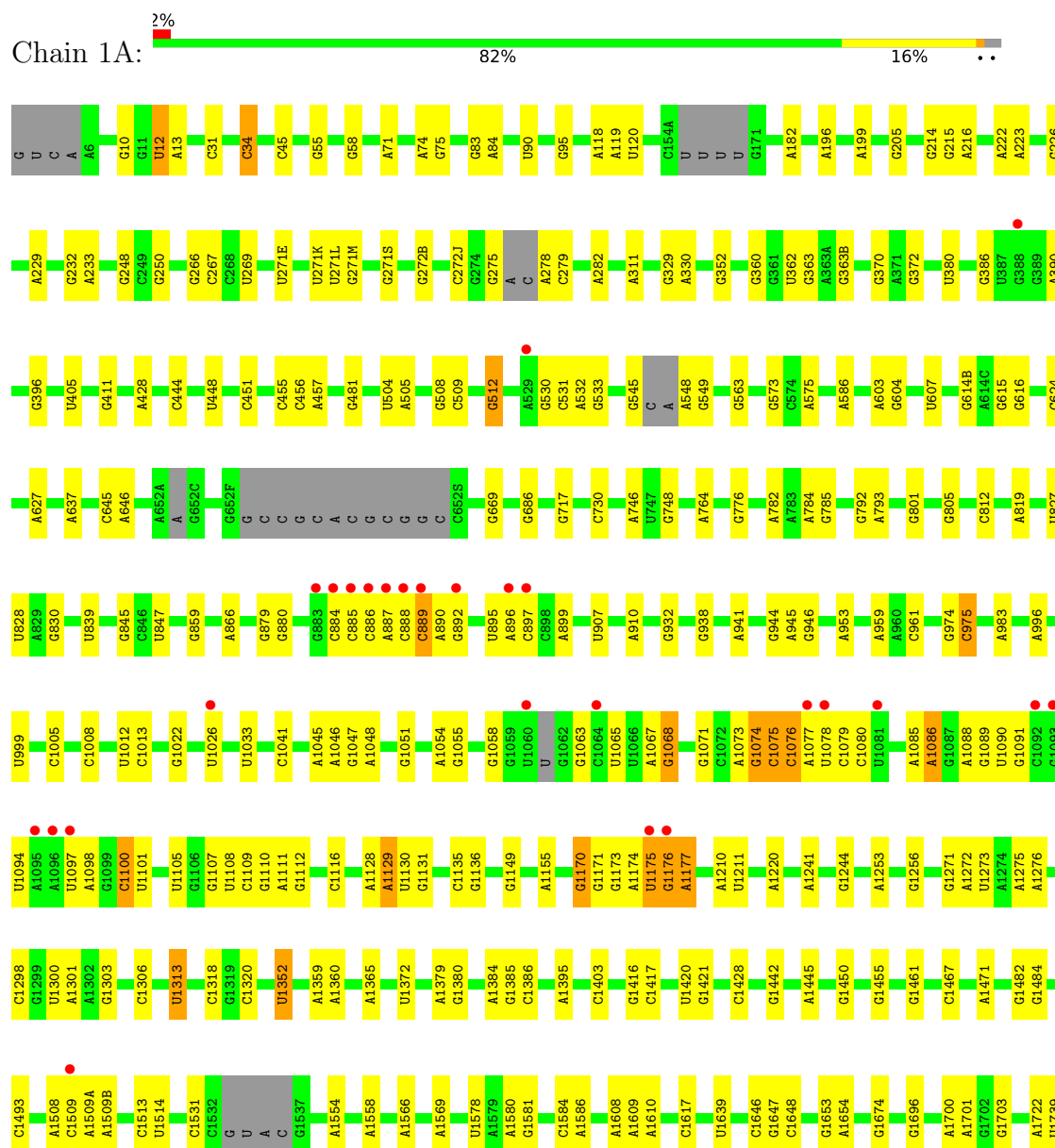
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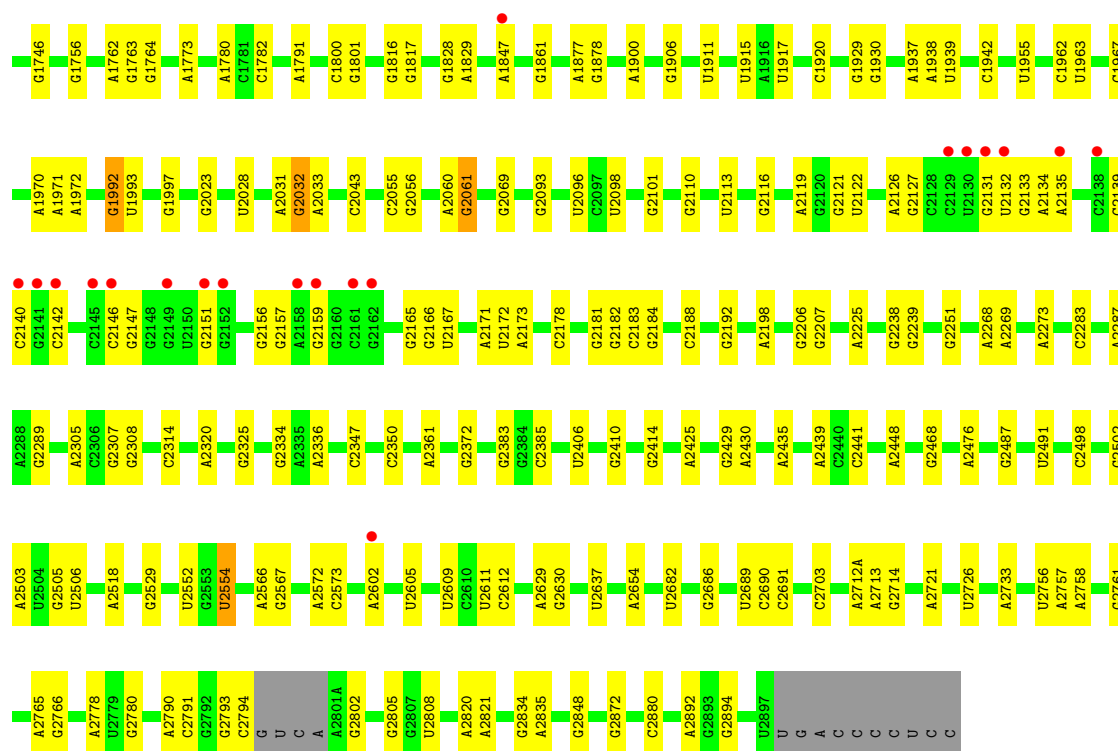
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	29	1	Total 1	O 1	0	0
62	2a	213	Total 213	O 213	0	0
62	2d	3	Total 3	O 3	0	0
62	2g	2	Total 2	O 2	0	0
62	2i	2	Total 2	O 2	0	0
62	2j	5	Total 5	O 5	0	0
62	2l	3	Total 3	O 3	0	0
62	2n	1	Total 1	O 1	0	0
62	2o	1	Total 1	O 1	0	0
62	2p	3	Total 3	O 3	0	0
62	2r	1	Total 1	O 1	0	0
62	2t	2	Total 2	O 2	0	0
62	2v	1	Total 1	O 1	0	0
62	2w	2	Total 2	O 2	0	0
62	2x	6	Total 6	O 6	0	0

3 Residue-property plots

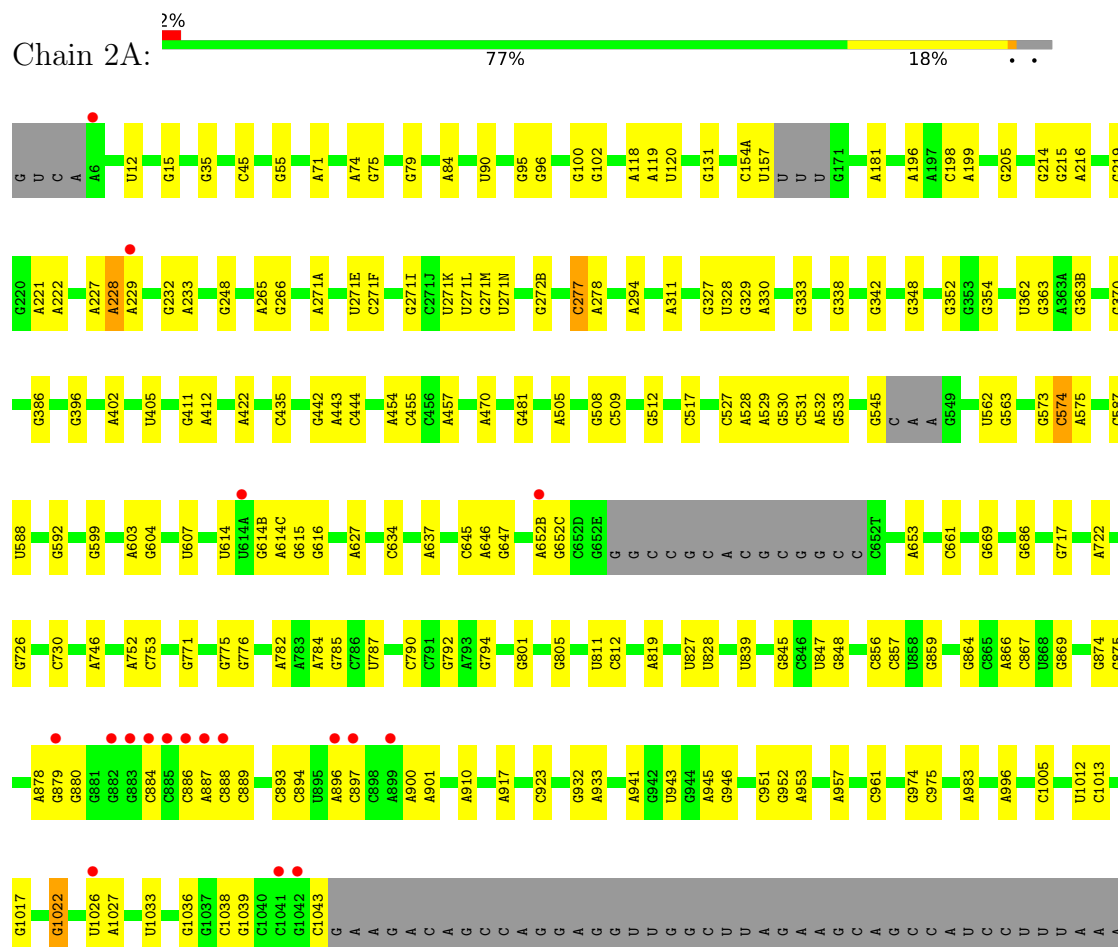
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: 23S Ribosomal RNA





• Molecule 1: 23S Ribosomal RNA



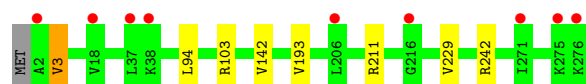




• Molecule 3: 50S Ribosomal Protein L2



• Molecule 3: 50S Ribosomal Protein L2



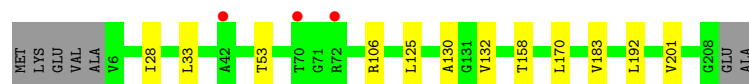
• Molecule 4: 50S Ribosomal Protein L3



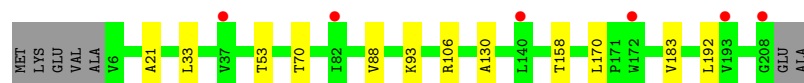
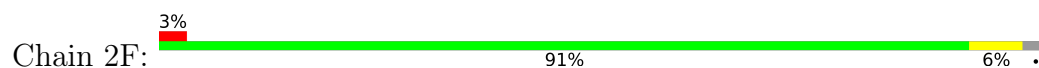
• Molecule 4: 50S Ribosomal Protein L3



• Molecule 5: 50S Ribosomal Protein L4

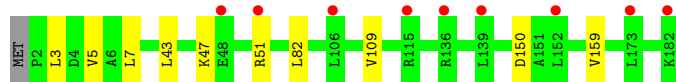


• Molecule 5: 50S Ribosomal Protein L4



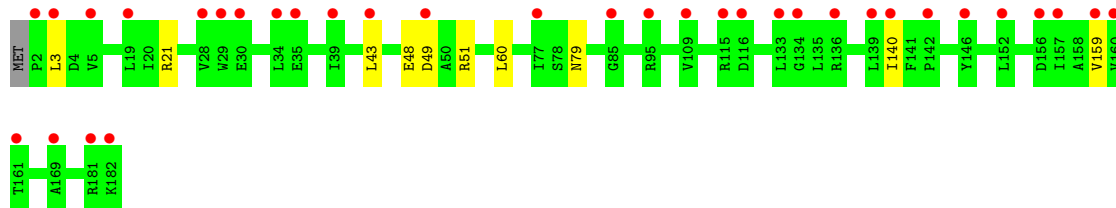
● Molecule 6: 50S Ribosomal Protein L5

Chain 1G:  5% 94% 5%



● Molecule 6: 50S Ribosomal Protein L5

Chain 2G:  19% 94% 5%



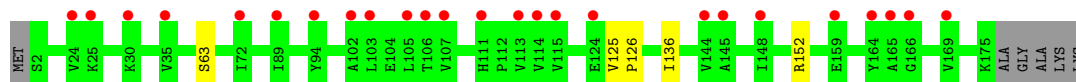
● Molecule 7: 50S Ribosomal Protein L6

Chain 1H:  2% 94% 5%




● Molecule 7: 50S Ribosomal Protein L6

Chain 2H:  14% 94% 5%

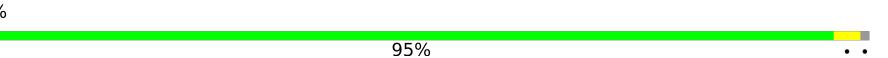


● Molecule 8: 50S Ribosomal Protein L9

Chain 1I:  % 93% 5%



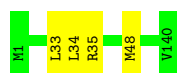
● Molecule 8: 50S Ribosomal Protein L9

Chain 2I:  % 95% 5%

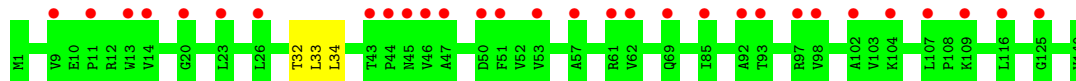


● Molecule 9: 50S Ribosomal Protein L13

Chain 1N:  97% 5%



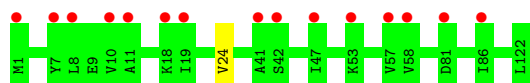
- Molecule 9: 50S Ribosomal Protein L13



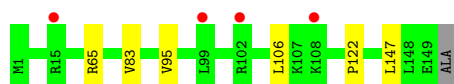
- Molecule 10: 50S Ribosomal Protein L14



- Molecule 10: 50S Ribosomal Protein L14



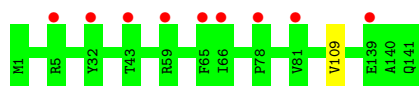
- Molecule 11: 50S Ribosomal Protein L15



- Molecule 11: 50S Ribosomal Protein L15

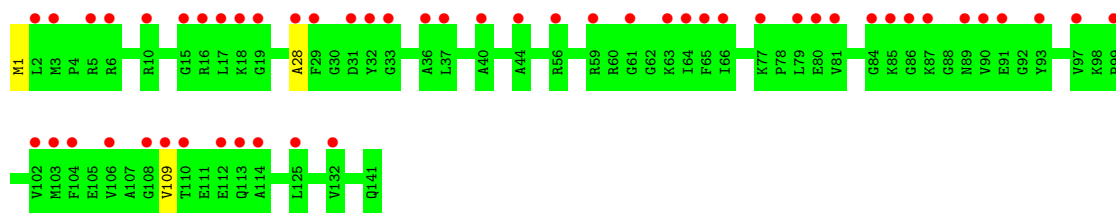


- Molecule 12: 50S Ribosomal Protein L16

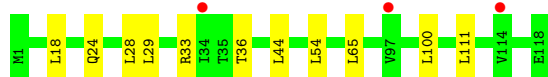


- Molecule 12: 50S Ribosomal Protein L16

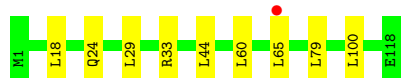




• Molecule 13: 50S Ribosomal Protein L17



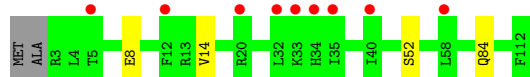
• Molecule 13: 50S Ribosomal Protein L17



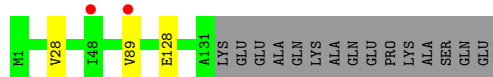
• Molecule 14: 50S Ribosomal Protein L18



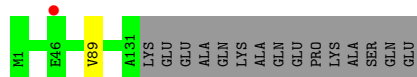
• Molecule 14: 50S Ribosomal Protein L18



• Molecule 15: 50S Ribosomal Protein L19

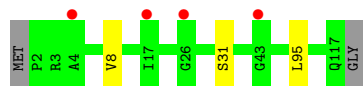


• Molecule 15: 50S Ribosomal Protein L19



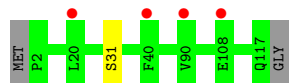
- Molecule 16: 50S Ribosomal Protein L20

Chain 1U:  96% ..



- Molecule 16: 50S Ribosomal Protein L20

Chain 2U:  97% ..



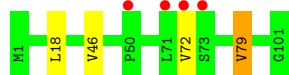
- Molecule 17: 50S Ribosomal Protein L21

Chain 1V:  93% 6% ..



- Molecule 17: 50S Ribosomal Protein L21

Chain 2V:  96% ..



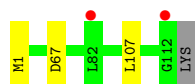
- Molecule 18: 50S Ribosomal Protein L22

Chain 1W:  96% ..



- Molecule 18: 50S Ribosomal Protein L22

Chain 2W:  96% ..

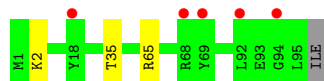


- Molecule 19: 50S Ribosomal Protein L23

Chain 1X:  97% ..



- Molecule 19: 50S Ribosomal Protein L23



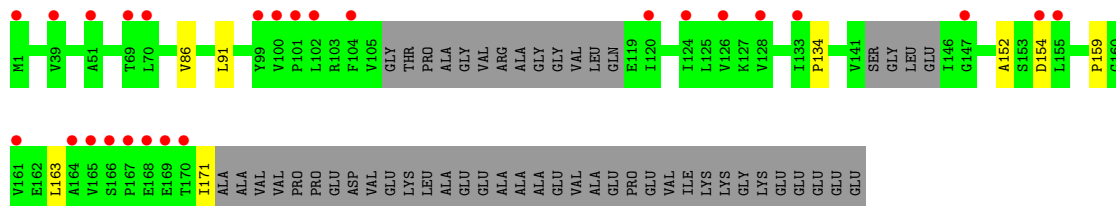
- Molecule 20: 50S Ribosomal Protein L24



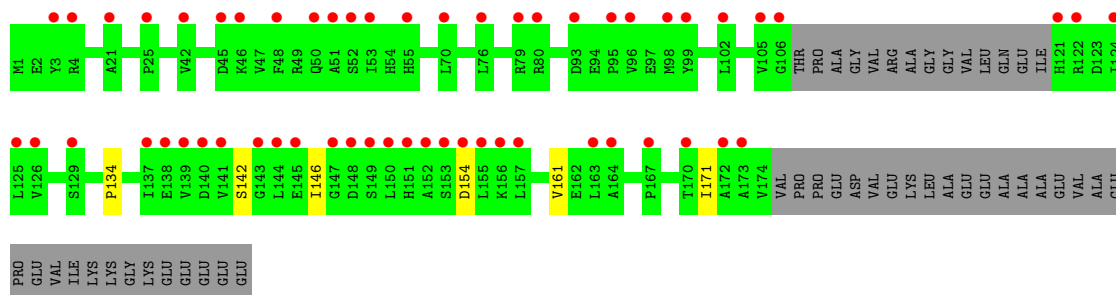
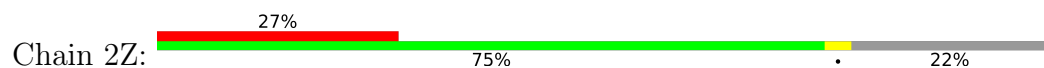
- Molecule 20: 50S Ribosomal Protein L24



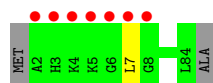
- Molecule 21: 50S Ribosomal Protein L25



- Molecule 21: 50S Ribosomal Protein L25

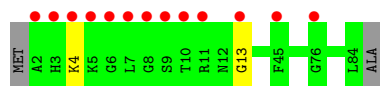


- Molecule 22: 50S Ribosomal Protein L27



- Molecule 22: 50S Ribosomal Protein L27

Chain 20:  15% 95% ..



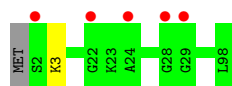
- Molecule 23: 50S Ribosomal Protein L28

Chain 11:  4% 97% ..



- Molecule 23: 50S Ribosomal Protein L28

Chain 21:  5% 98% ..



- Molecule 24: 50S Ribosomal Protein L29

Chain 12:  96% ..



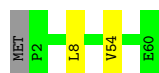
- Molecule 24: 50S Ribosomal Protein L29

Chain 22:  94% ..



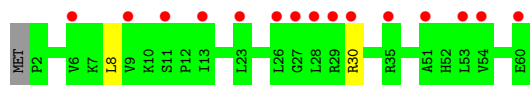
- Molecule 25: 50S Ribosomal Protein L30

Chain 13:  95% ..

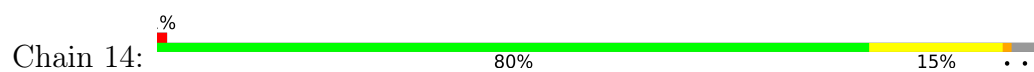


- Molecule 25: 50S Ribosomal Protein L30

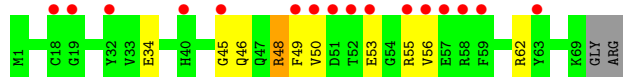
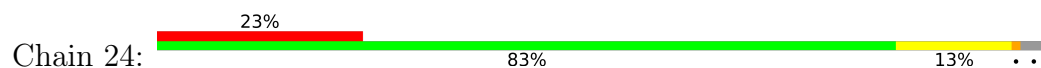
Chain 23:  25% 95% ..



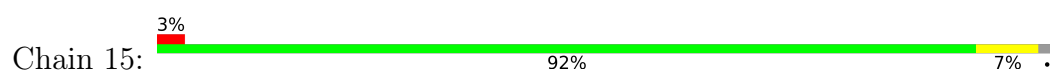
- Molecule 26: 50S Ribosomal Protein L31



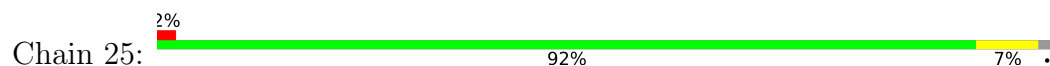
• Molecule 26: 50S Ribosomal Protein L31



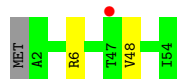
• Molecule 27: 50S Ribosomal Protein L32



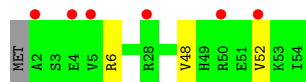
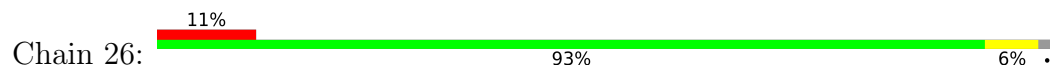
• Molecule 27: 50S Ribosomal Protein L32



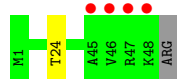
• Molecule 28: 50S Ribosomal Protein L33



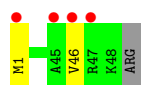
• Molecule 28: 50S Ribosomal Protein L33



• Molecule 29: 50S Ribosomal Protein L34



• Molecule 29: 50S Ribosomal Protein L34



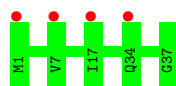
- Molecule 30: 50S Ribosomal Protein L35



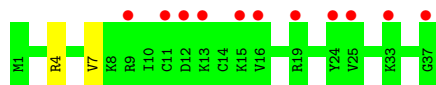
- Molecule 30: 50S Ribosomal Protein L35



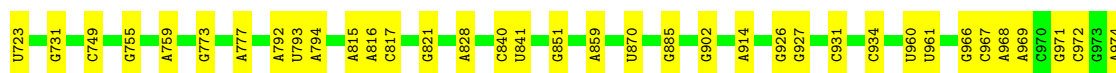
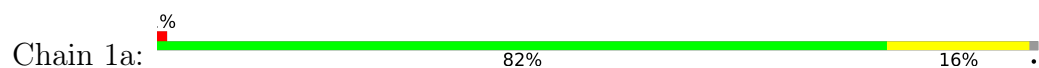
- Molecule 31: 50S Ribosomal Protein L36

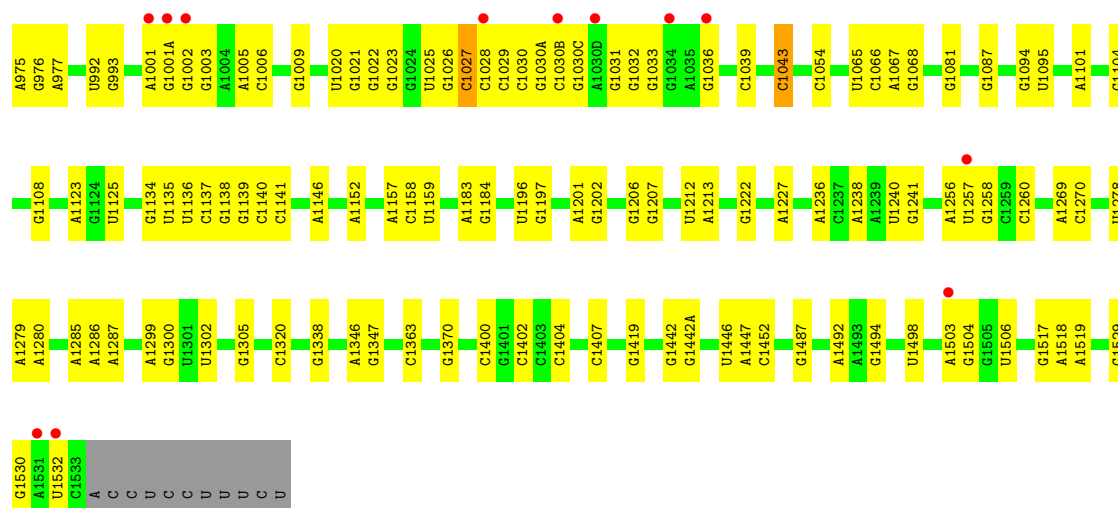


- Molecule 31: 50S Ribosomal Protein L36

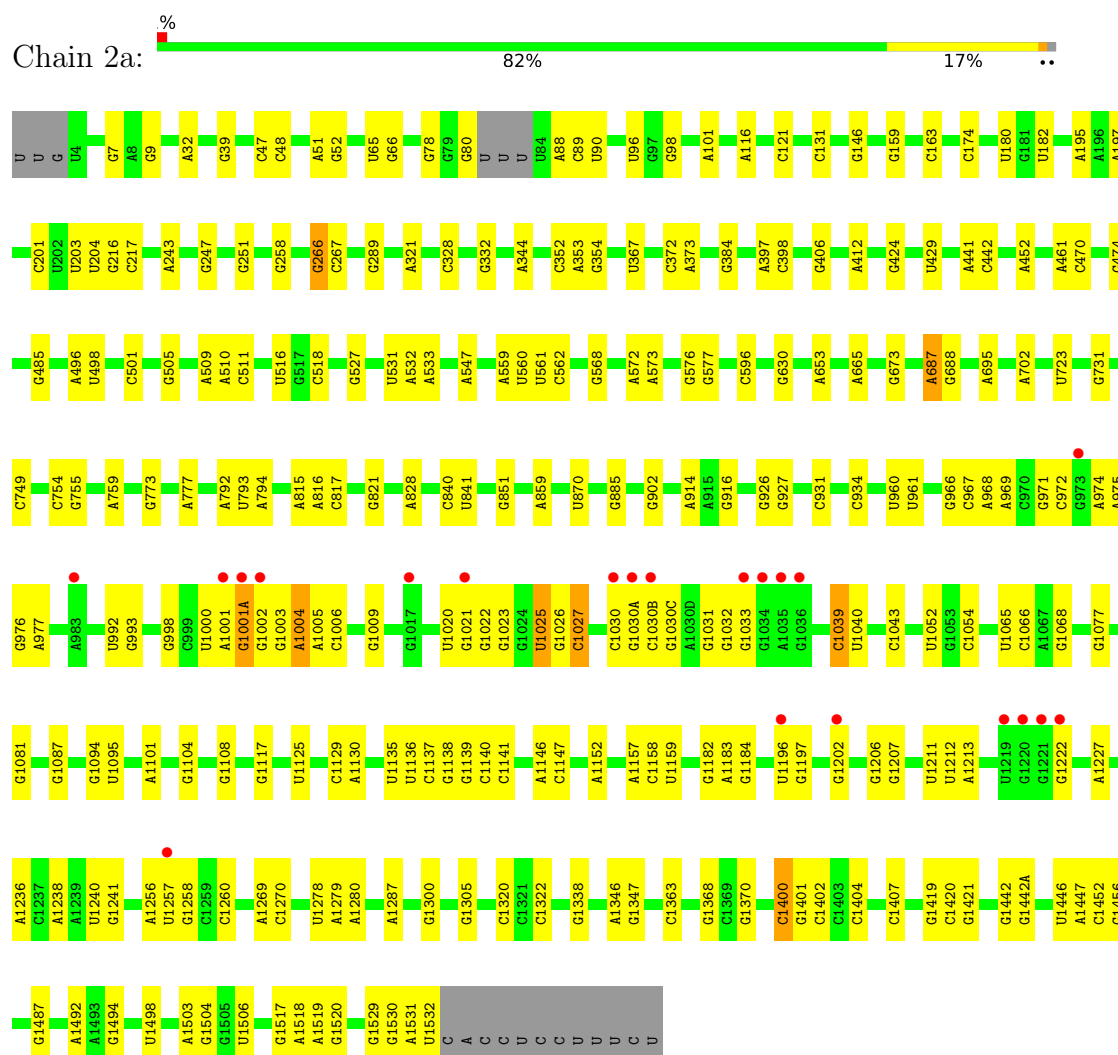


- Molecule 32: 16S Ribosomal RNA



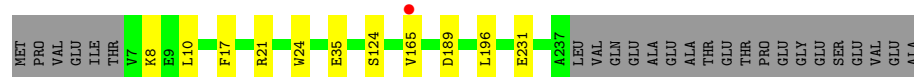


• Molecule 32: 16S Ribosomal RNA

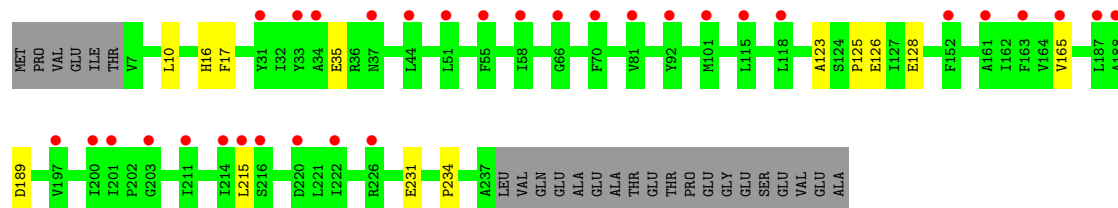
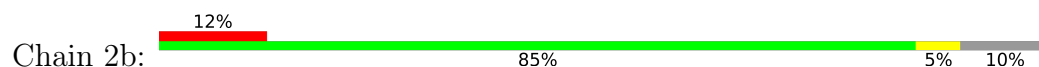


• Molecule 33: 30S Ribosomal Protein S2

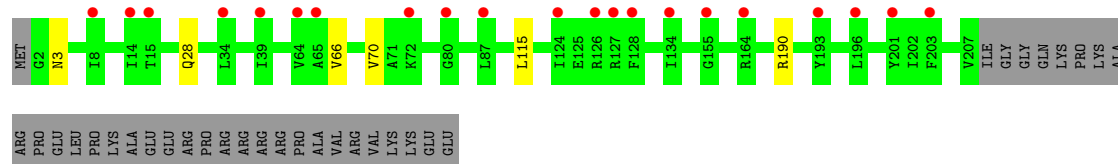
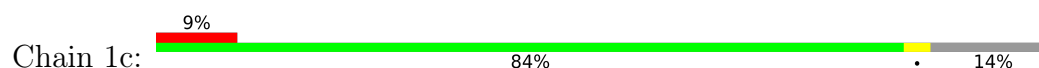




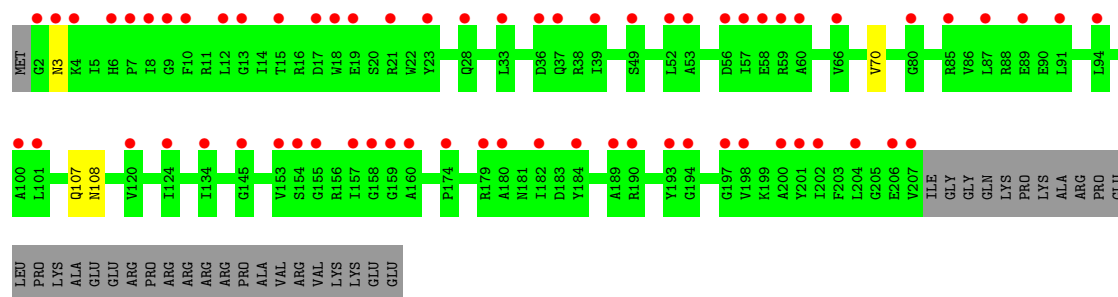
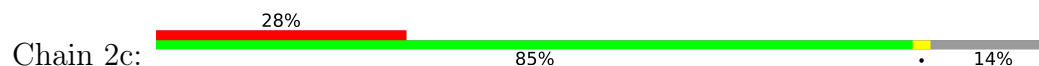
• Molecule 33: 30S Ribosomal Protein S2



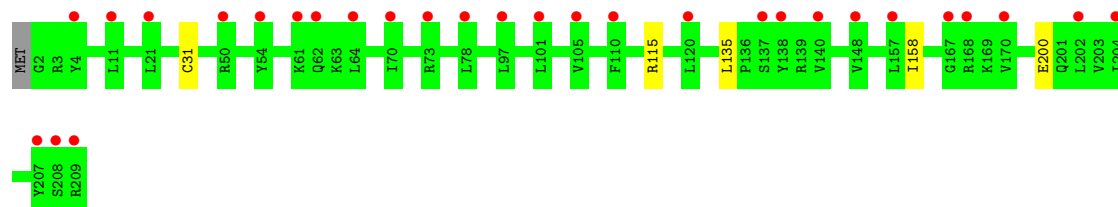
• Molecule 34: 30S Ribosomal Protein S3



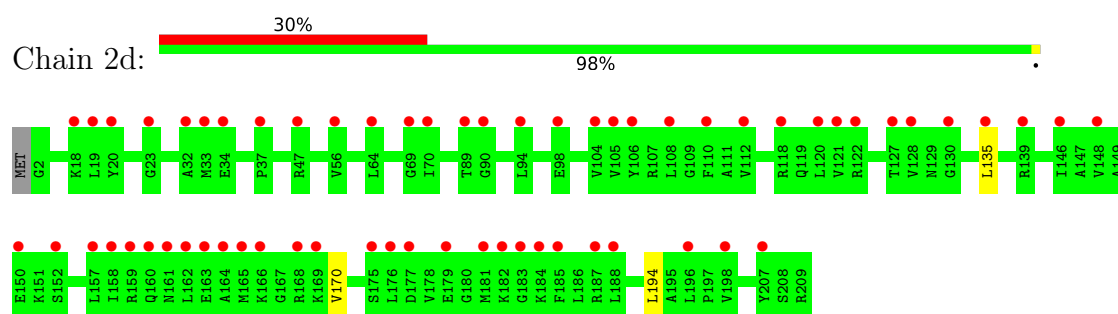
• Molecule 34: 30S Ribosomal Protein S3



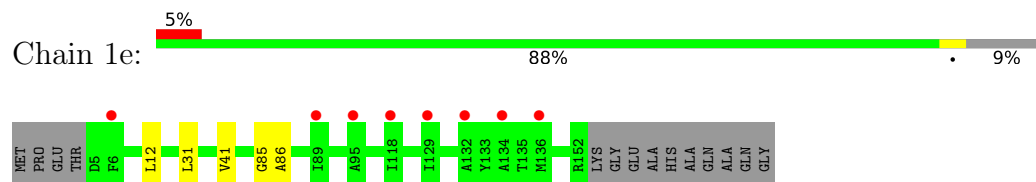
• Molecule 35: 30S Ribosomal Protein S4



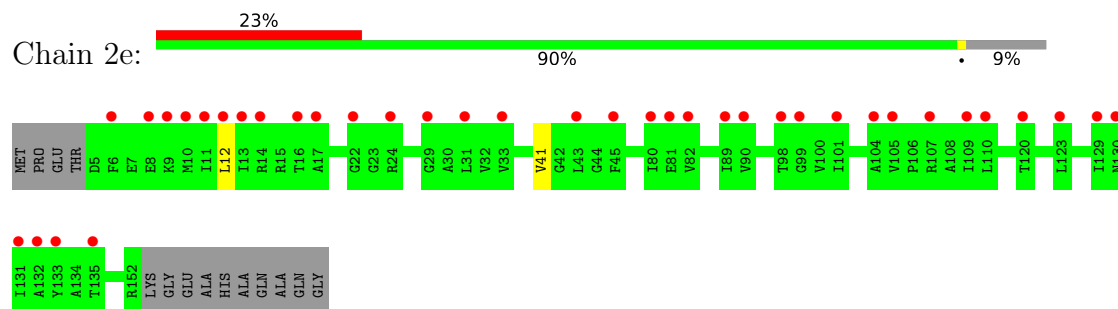
• Molecule 35: 30S Ribosomal Protein S4



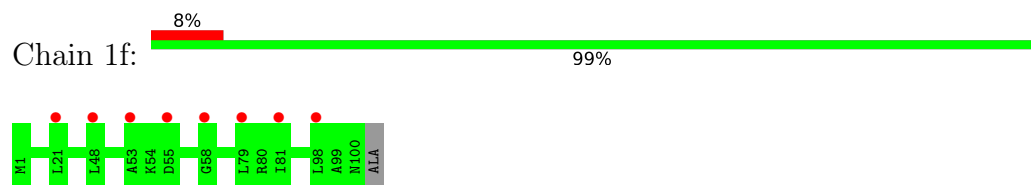
- Molecule 36: 30S Ribosomal Protein S5



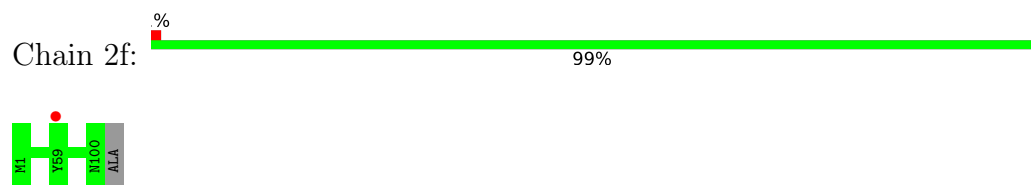
- Molecule 36: 30S Ribosomal Protein S5



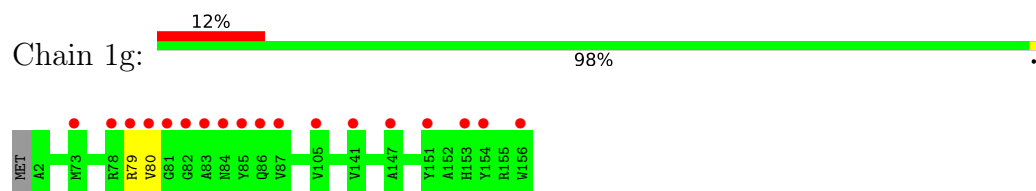
- Molecule 37: 30S Ribosomal Protein S6



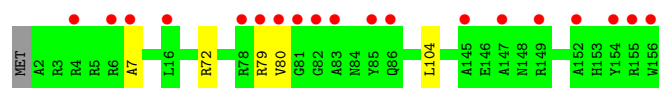
- Molecule 37: 30S Ribosomal Protein S6



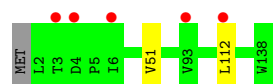
- Molecule 38: 30S Ribosomal Protein S7



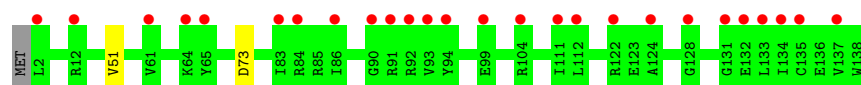
- Molecule 38: 30S Ribosomal Protein S7



- Molecule 39: 30S Ribosomal Protein S8



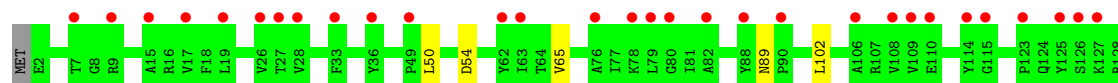
- Molecule 39: 30S Ribosomal Protein S8



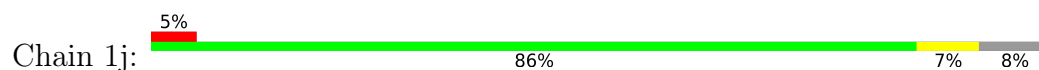
- Molecule 40: 30S Ribosomal Protein S9



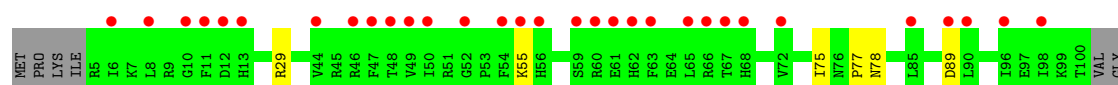
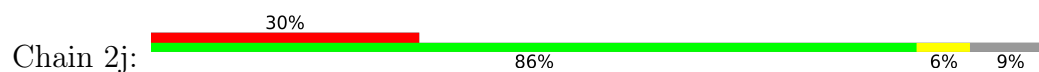
- Molecule 40: 30S Ribosomal Protein S9



- Molecule 41: 30S Ribosomal Protein S10




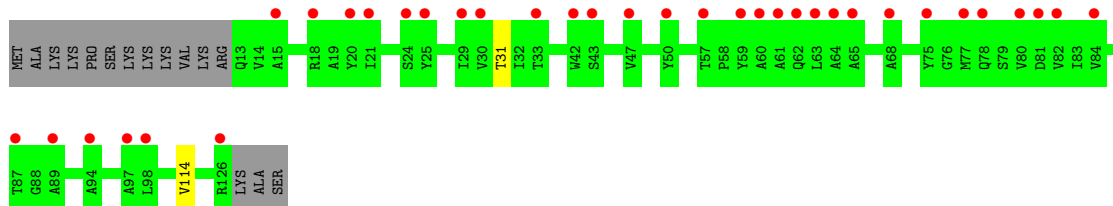
- Molecule 41: 30S Ribosomal Protein S10




GLY
GLY
ARG

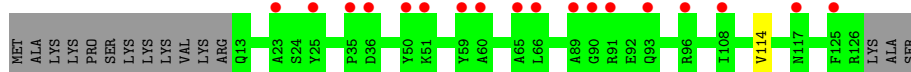
• Molecule 42: 30S Ribosomal Protein S11

Chain 1k:  27% 87% 12%




• Molecule 42: 30S Ribosomal Protein S11

Chain 2k:  14% 88% 12%




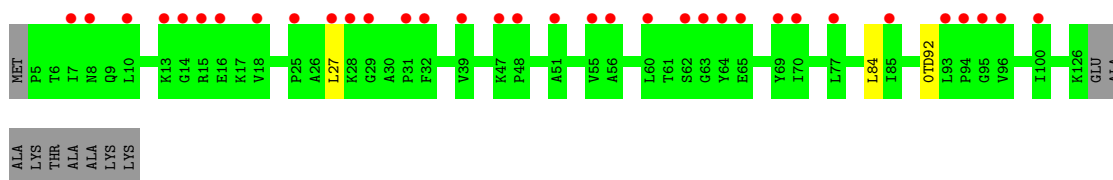
• Molecule 43: 30S Ribosomal Protein S12

Chain 1l:  4% 89% 8%



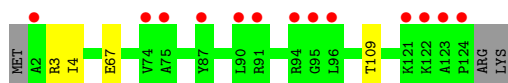
• Molecule 43: 30S Ribosomal Protein S12

Chain 2l:  26% 90% 8%



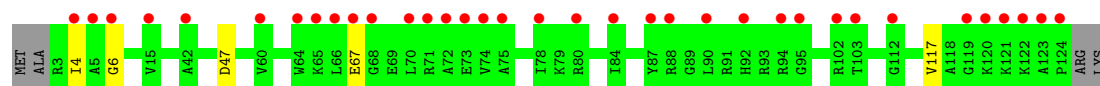
• Molecule 44: 30S Ribosomal Protein S13

Chain 1m:  10% 94% 2%



• Molecule 44: 30S Ribosomal Protein S13

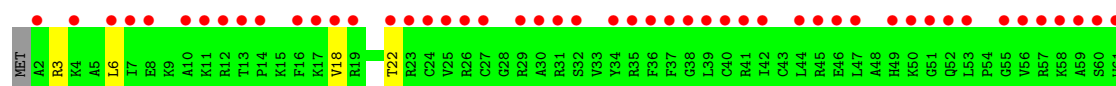
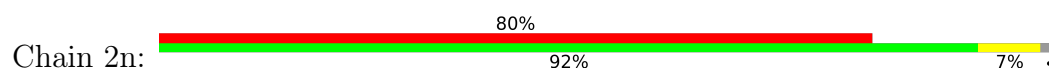
Chain 2m:  28% 93% 2%



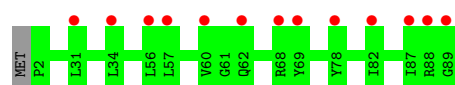
• Molecule 45: 30S Ribosomal Protein S14



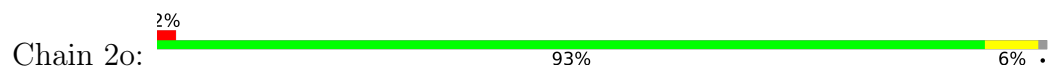
• Molecule 45: 30S Ribosomal Protein S14



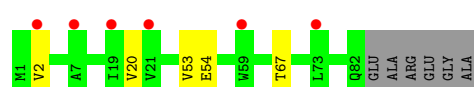
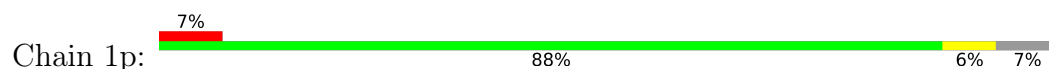
• Molecule 46: 30S Ribosomal Protein S15



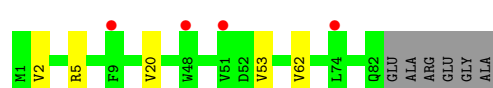
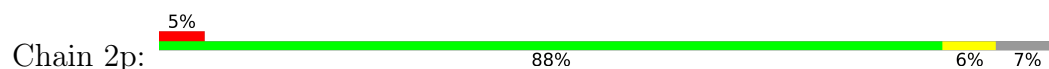
• Molecule 46: 30S Ribosomal Protein S15



• Molecule 47: 30S Ribosomal Protein S16



• Molecule 47: 30S Ribosomal Protein S16

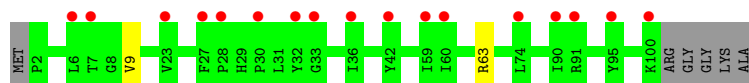
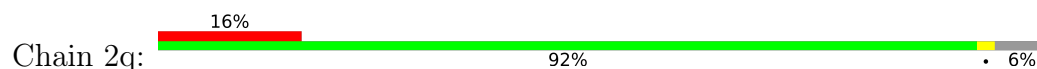


• Molecule 48: 30S Ribosomal Protein S17

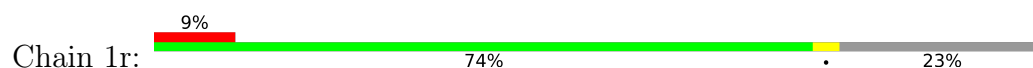




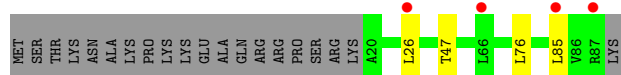
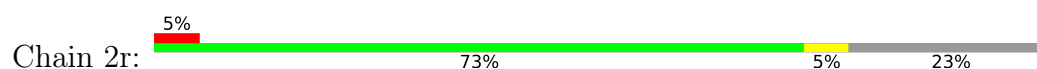
• Molecule 48: 30S Ribosomal Protein S17



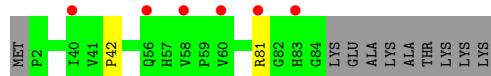
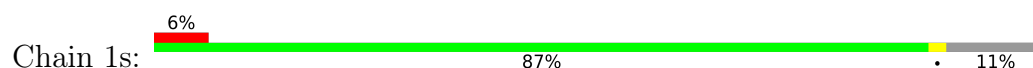
• Molecule 49: 30S Ribosomal Protein S18



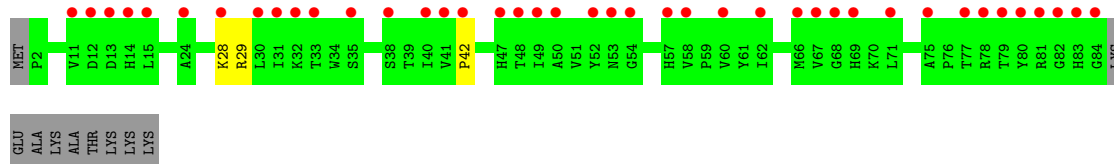
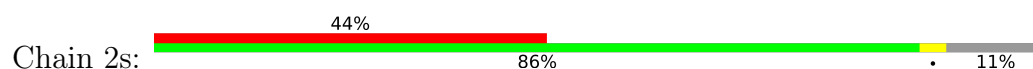
• Molecule 49: 30S Ribosomal Protein S18



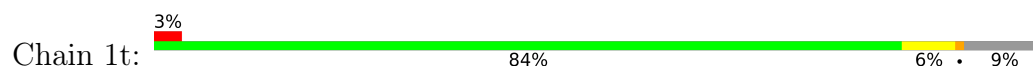
• Molecule 50: 30S Ribosomal Protein S19



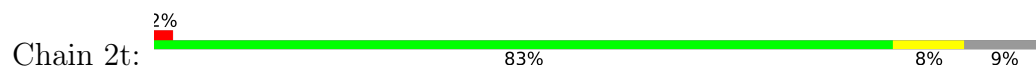
• Molecule 50: 30S Ribosomal Protein S19



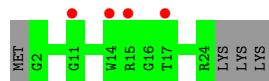
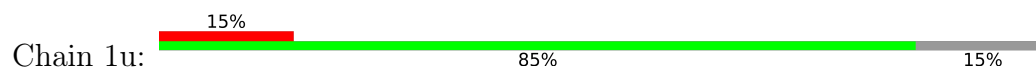
• Molecule 51: 30S Ribosomal Protein S20



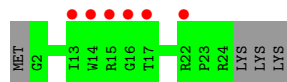
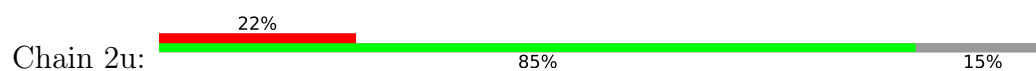
- Molecule 51: 30S Ribosomal Protein S20



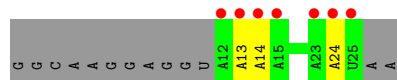
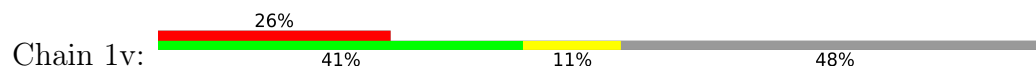
- Molecule 52: 30S Ribosomal Protein THX



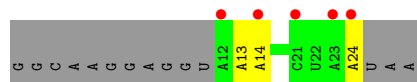
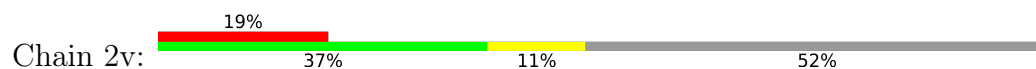
- Molecule 52: 30S Ribosomal Protein THX



- Molecule 53: mRNA



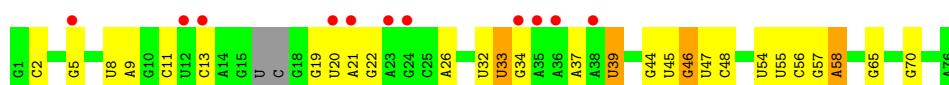
- Molecule 53: mRNA



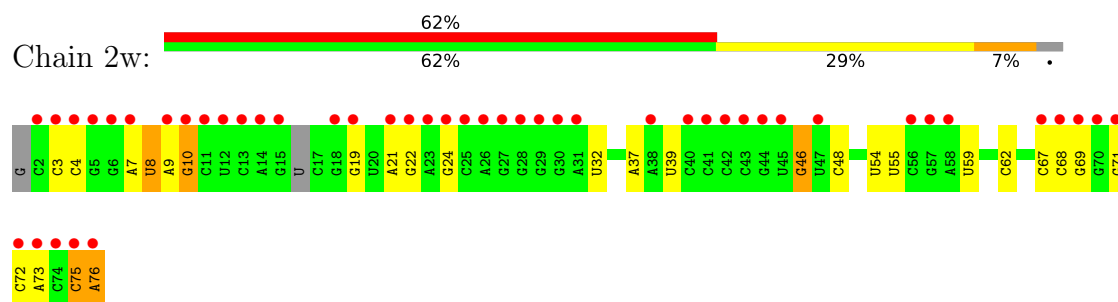
- Molecule 54: A-site and E-site tRNAs



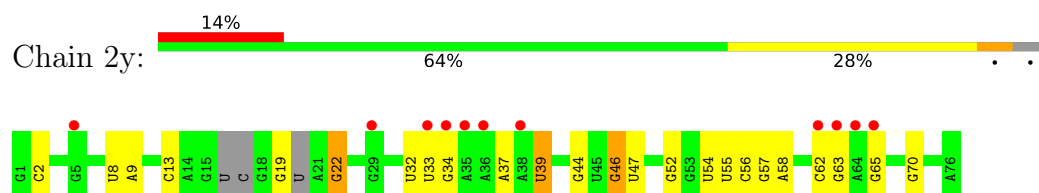
- Molecule 54: A-site and E-site tRNAs



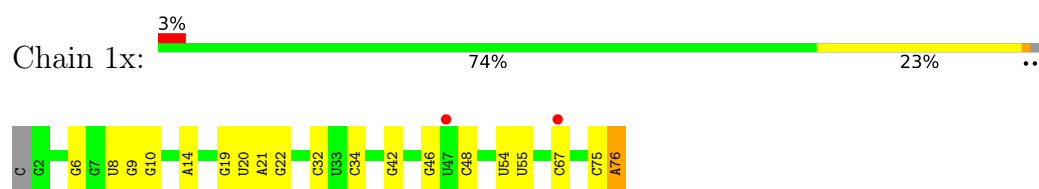
- Molecule 54: A-site and E-site tRNAs



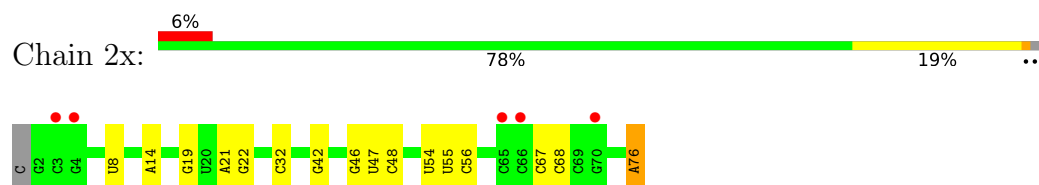
- Molecule 54: A-site and E-site tRNAs



- Molecule 55: P-site tRNA



- Molecule 55: P-site tRNA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	208.39Å 444.58Å 619.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	361.14 – 2.60 361.14 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.3 (361.14-2.60) 99.3 (361.14-2.60)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 2.62Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.233 , 0.283 0.233 , 0.283	Depositor DCC
R_{free} test set	86608 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	51.7	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 61.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	298925	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.63% 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: FME, 4OC, 2MA, UR3, 2MU, K, M2G, ZN, HGR, MIA, 4SU, 5MC, 2MG, SF4, 5MU, OMG, MA6, 0TD, 7MG, MG, 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	0.52	0/69009	0.95	67/107712 (0.1%)
1	2A	0.43	0/67293	0.93	46/105034 (0.0%)
2	1B	0.46	1/2882 (0.0%)	0.85	0/4494
2	2B	0.49	1/2879 (0.0%)	0.93	2/4487 (0.0%)
3	1D	0.38	0/2186	0.59	0/2944
3	2D	0.34	0/2186	0.59	0/2944
4	1E	0.37	0/1592	0.57	0/2149
4	2E	0.33	0/1592	0.56	1/2149 (0.0%)
5	1F	0.36	0/1619	0.55	0/2193
5	2F	0.33	0/1615	0.56	0/2188
6	1G	0.32	0/1454	0.53	0/1964
6	2G	0.31	0/1453	0.56	0/1963
7	1H	0.33	0/1356	0.52	0/1834
7	2H	0.29	0/1356	0.52	0/1834
8	1I	0.29	0/1112	0.54	0/1514
8	2I	0.28	0/1079	0.54	0/1475
9	1N	0.34	0/1144	0.55	0/1543
9	2N	0.28	0/1144	0.53	0/1543
10	1O	0.37	0/943	0.55	0/1269
10	2O	0.33	0/943	0.52	0/1269
11	1P	0.35	0/1152	0.55	0/1533
11	2P	0.32	0/1152	0.60	0/1533
12	1Q	0.39	0/1143	0.54	0/1527
12	2Q	0.33	0/1143	0.58	0/1527
13	1R	0.37	0/982	0.59	0/1312
13	2R	0.33	0/982	0.56	0/1312
14	1S	0.32	0/883	0.53	0/1176
14	2S	0.32	0/880	0.57	0/1172
15	1T	0.34	0/1105	0.52	0/1477
15	2T	0.31	0/1097	0.53	0/1468
16	1U	0.41	0/977	0.55	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.34	0/977	0.53	0/1301
17	1V	0.39	0/782	0.54	0/1049
17	2V	0.33	0/782	0.53	0/1049
18	1W	0.40	0/897	0.56	0/1205
18	2W	0.34	0/897	0.52	0/1205
19	1X	0.41	0/764	0.59	0/1025
19	2X	0.34	0/764	0.53	0/1025
20	1Y	0.35	0/819	0.55	0/1095
20	2Y	0.32	0/819	0.55	0/1095
21	1Z	0.32	0/1267	0.54	0/1717
21	2Z	0.28	0/1299	0.53	0/1763
22	10	0.38	0/662	0.57	0/881
22	20	0.31	0/662	0.54	0/881
23	11	0.35	0/762	0.54	0/1014
23	21	0.32	0/762	0.53	0/1014
24	12	0.31	0/590	0.53	0/781
24	22	0.29	0/590	0.45	0/781
25	13	0.34	0/474	0.53	0/635
25	23	0.30	0/469	0.52	0/630
26	14	0.34	0/565	0.66	0/761
26	24	0.31	0/545	0.66	0/737
27	15	0.39	0/469	0.62	0/635
27	25	0.31	0/469	0.57	1/635 (0.2%)
28	16	0.38	0/460	0.54	0/613
28	26	0.31	0/456	0.51	0/608
29	17	0.39	0/426	0.54	0/561
29	27	0.32	0/426	0.54	0/561
30	18	0.38	0/525	0.56	0/691
30	28	0.33	0/525	0.53	0/691
31	19	0.36	0/310	0.50	0/407
31	29	0.32	0/310	0.58	0/407
32	1a	0.38	0/35795	0.88	27/55864 (0.0%)
32	2a	0.37	0/35886	0.91	33/56005 (0.1%)
33	1b	0.29	0/1881	0.59	0/2542
33	2b	0.31	0/1860	0.57	0/2518
34	1c	0.28	0/1572	0.52	2/2126 (0.1%)
34	2c	0.29	0/1566	0.55	0/2119
35	1d	0.28	0/1685	0.51	0/2262
35	2d	0.28	0/1704	0.49	0/2284
36	1e	0.31	0/1145	0.54	0/1543
36	2e	0.29	0/1149	0.57	0/1548
37	1f	0.30	0/823	0.50	0/1115
37	2f	0.30	0/829	0.48	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.29	0/1250	0.53	0/1679
38	2g	0.29	0/1254	0.55	0/1683
39	1h	0.27	0/1108	0.54	0/1494
39	2h	0.27	0/1108	0.54	0/1494
40	1i	0.28	0/1002	0.57	1/1346 (0.1%)
40	2i	0.28	0/997	0.56	0/1343
41	1j	0.27	0/722	0.53	0/982
41	2j	0.29	0/727	0.56	0/988
42	1k	0.28	0/844	0.52	0/1145
42	2k	0.27	0/848	0.48	0/1149
43	1l	0.32	0/937	0.53	0/1260
43	2l	0.30	0/937	0.56	0/1260
44	1m	0.29	0/969	0.54	0/1302
44	2m	0.30	0/961	0.56	0/1291
45	1n	0.31	0/501	0.48	0/664
45	2n	0.29	0/501	0.48	0/664
46	1o	0.29	0/739	0.52	0/985
46	2o	0.27	0/739	0.54	0/985
47	1p	0.28	0/697	0.52	0/939
47	2p	0.29	0/693	0.52	0/935
48	1q	0.29	0/836	0.51	0/1117
48	2q	0.28	0/836	0.52	0/1117
49	1r	0.29	0/560	0.49	0/746
49	2r	0.28	0/560	0.52	0/746
50	1s	0.28	0/667	0.56	0/900
50	2s	0.32	0/661	0.62	0/893
51	1t	0.27	0/730	0.52	0/965
51	2t	0.27	0/729	0.53	0/965
52	1u	0.27	0/203	0.47	0/266
52	2u	0.30	0/203	0.50	0/266
53	1v	0.40	0/314	0.90	0/487
53	2v	0.40	0/310	0.87	0/480
54	1w	0.45	0/1585	1.14	11/2468 (0.4%)
54	1y	0.39	0/1602	1.02	3/2493 (0.1%)
54	2w	0.52	0/1562	1.21	5/2431 (0.2%)
54	2y	0.46	0/1579	1.10	4/2455 (0.2%)
55	1x	0.79	7/1725 (0.4%)	1.34	31/2689 (1.2%)
55	2x	0.61	4/1725 (0.2%)	1.30	17/2689 (0.6%)
All	All	0.42	13/316673 (0.0%)	0.85	251/474103 (0.1%)

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
26	14	0	1
50	2s	0	1
All	All	0	2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	1x	76	A	N7-C5	-19.10	1.27	1.39
55	2x	76	A	N7-C5	-11.09	1.32	1.39
2	2B	1	U	OP3-P	-10.32	1.48	1.61
2	1B	1	U	OP3-P	-10.29	1.48	1.61
55	2x	76	A	C5-C6	-8.01	1.33	1.41
55	2x	76	A	C5-C4	-7.80	1.33	1.38
55	1x	76	A	N9-C8	-7.74	1.31	1.37
55	1x	76	A	C5-C4	-7.49	1.33	1.38
55	1x	22	G	N7-C5	7.16	1.43	1.39
55	1x	76	A	N9-C4	-6.87	1.33	1.37
55	1x	76	A	C5-C6	-6.78	1.34	1.41
55	2x	76	A	N9-C4	-5.29	1.34	1.37
55	1x	46	G	C6-N1	5.15	1.43	1.39

All (251) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	1x	76	A	N1-C2-N3	-19.21	119.69	129.30
55	2x	76	A	N1-C2-N3	-18.82	119.89	129.30
55	2x	76	A	C2-N3-C4	18.77	119.99	110.60
55	1x	76	A	C2-N3-C4	18.41	119.80	110.60
55	2x	76	A	O4'-C1'-N9	15.30	120.44	108.20
2	2B	80	U	O4'-C1'-N1	11.58	117.47	108.20
32	2a	1420	C	OP1-P-O3'	-11.56	79.77	105.20
55	1x	46	G	C6-N1-C2	-10.60	118.74	125.10
32	1a	1027	C	C2-N1-C1'	10.47	130.32	118.80
1	1A	975	C	N1-C2-O2	-10.11	112.83	118.90
55	2x	76	A	N3-C4-C5	-9.96	119.83	126.80
1	1A	1075	C	N1-C2-O2	9.84	124.81	118.90
54	1w	72	C	C2-N1-C1'	9.59	129.35	118.80
55	1x	75	C	OP1-P-O3'	-9.47	84.37	105.20
1	2A	2139	C	N1-C2-O2	9.40	124.54	118.90
55	1x	75	C	OP2-P-O3'	9.35	125.76	105.20
55	2x	76	A	N7-C8-N9	-9.22	109.19	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1036	G	C4-N9-C1'	9.17	138.42	126.50
55	1x	76	A	N3-C4-C5	-9.16	120.39	126.80
32	2a	1420	C	OP2-P-O3'	-9.07	85.23	105.20
1	2A	2061	G	O5'-P-OP2	-9.01	97.59	105.70
1	2A	277	C	N1-C2-O2	9.00	124.30	118.90
32	1a	1030(B)	C	C2-N1-C1'	8.99	128.69	118.80
32	1a	1027	C	C6-N1-C1'	-8.86	110.17	120.80
1	2A	801	G	O5'-P-OP2	-8.68	97.89	105.70
55	1x	76	A	N7-C8-N9	-8.62	109.49	113.80
55	1x	76	A	C5-N7-C8	8.59	108.20	103.90
32	1a	1036	G	C8-N9-C1'	-8.31	116.19	127.00
55	1x	22	G	C4-C5-C6	-8.30	113.82	118.80
55	1x	22	G	N1-C6-O6	-8.23	114.96	119.90
55	2x	76	A	C5-N7-C8	8.17	107.99	103.90
1	1A	975	C	C2-N1-C1'	-8.13	109.86	118.80
1	1A	1063	G	C5-C6-O6	7.97	133.38	128.60
55	2x	76	A	N9-C4-C5	7.94	108.97	105.80
1	2A	277	C	C2-N1-C1'	7.92	127.52	118.80
54	1w	1	G	N3-C4-N9	7.81	130.69	126.00
1	1A	2167	U	C2-N1-C1'	7.74	126.99	117.70
1	2A	2167	U	N3-C2-O2	-7.73	116.79	122.20
55	2x	14	A	C4-C5-C6	7.71	120.85	117.00
1	1A	801	G	O5'-P-OP2	-7.68	98.78	105.70
1	1A	512	G	O4'-C1'-N9	7.61	114.29	108.20
1	1A	2682	U	O5'-P-OP2	-7.59	98.87	105.70
1	2A	2136	C	N1-C2-O2	7.58	123.45	118.90
54	1w	72	C	C6-N1-C1'	-7.56	111.72	120.80
32	1a	1030(B)	C	N1-C2-O2	7.54	123.42	118.90
1	1A	1639	U	O5'-P-OP2	-7.39	99.05	105.70
55	1x	22	G	C5-N7-C8	-7.38	100.61	104.30
32	2a	1004	A	O4'-C1'-N9	7.34	114.07	108.20
1	1A	12	U	C2-N1-C1'	7.32	126.48	117.70
32	2a	1001(A)	G	N3-C4-N9	7.26	130.35	126.00
1	2A	2139	C	C2-N1-C1'	7.25	126.77	118.80
1	2A	2167	U	N1-C2-O2	7.24	127.87	122.80
32	2a	1421	G	OP1-P-OP2	7.13	130.29	119.60
1	2A	277	C	N3-C2-O2	-7.10	116.93	121.90
1	1A	1075	C	C2-N3-C4	7.09	123.45	119.90
1	2A	2167	U	C2-N1-C1'	7.05	126.16	117.70
1	1A	1100	C	C2-N1-C1'	7.02	126.52	118.80
55	2x	76	A	C4-C5-C6	7.01	120.51	117.00
54	1w	72	C	N1-C2-O2	7.00	123.10	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	2x	46	G	C6-N1-C2	-7.00	120.90	125.10
55	1x	22	G	N3-C4-N9	-6.99	121.81	126.00
32	1a	1027	C	C5-C6-N1	6.94	124.47	121.00
55	1x	22	G	C6-C5-N7	6.90	134.54	130.40
55	1x	14	A	C4-C5-C6	6.85	120.43	117.00
1	1A	1992	G	P-O3'-C3'	6.76	127.81	119.70
1	1A	1086	A	N1-C6-N6	-6.72	114.57	118.60
55	1x	76	A	N9-C4-C5	6.69	108.48	105.80
55	1x	76	A	C5-C6-N1	6.63	121.02	117.70
1	1A	793	A	O5'-P-OP2	-6.61	99.75	105.70
32	1a	1002	G	N3-C4-N9	6.61	129.96	126.00
1	1A	1176	G	OP1-P-O3'	6.58	119.68	105.20
32	1a	1036	G	N3-C4-N9	6.55	129.93	126.00
1	1A	1075	C	N3-C2-O2	-6.54	117.33	121.90
1	2A	1022	G	N3-C4-N9	-6.53	122.08	126.00
1	1A	2167	U	N1-C2-O2	6.46	127.32	122.80
1	1A	847	U	C2-N1-C1'	6.45	125.43	117.70
1	2A	574	C	O5'-P-OP1	-6.44	99.91	105.70
32	2a	998	G	N9-C4-C5	6.42	107.97	105.40
1	1A	2848	G	O4'-C1'-N9	6.38	113.31	108.20
55	1x	14	A	C5-N7-C8	6.38	107.09	103.90
54	2y	63	G	C5-C6-O6	6.38	132.43	128.60
1	1A	975	C	C5-C6-N1	-6.31	117.84	121.00
1	1A	1298	C	O5'-P-OP2	-6.29	100.04	105.70
32	1a	1030(B)	C	C6-N1-C2	-6.29	117.78	120.30
55	2x	14	A	C5-N7-C8	6.24	107.02	103.90
1	1A	2167	U	N3-C2-O2	-6.22	117.84	122.20
32	2a	998	G	N3-C4-N9	-6.22	122.27	126.00
1	2A	277	C	C6-N1-C2	-6.17	117.83	120.30
1	1A	624	C	O5'-P-OP1	-6.17	100.15	105.70
1	1A	1063	G	C6-N1-C2	6.16	128.80	125.10
1	2A	2139	C	C6-N1-C1'	-6.16	113.41	120.80
1	2A	2554	U	O5'-P-OP2	-6.15	100.16	105.70
32	2a	1322	C	N1-C2-O2	-6.15	115.21	118.90
32	1a	1030(B)	C	C6-N1-C1'	-6.14	113.44	120.80
27	25	58	LEU	CA-CB-CG	6.13	129.41	115.30
32	1a	1036	G	N3-C4-C5	-6.10	125.55	128.60
1	2A	2155	G	N3-C2-N2	6.07	124.15	119.90
32	1a	1002	G	C4-N9-C1'	6.06	134.38	126.50
1	1A	975	C	C6-N1-C1'	6.04	128.05	120.80
1	2A	1300	U	P-O3'-C3'	6.04	126.94	119.70
1	2A	2897	U	C2-N1-C1'	6.04	124.94	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	1x	22	G	C8-N9-C1'	6.03	134.84	127.00
1	1A	1129	A	O4'-C1'-N9	6.00	113.00	108.20
32	2a	754	C	C2-N1-C1'	5.98	125.38	118.80
1	1A	31	C	O5'-P-OP1	-5.95	100.35	105.70
1	2A	2206	G	C4-N9-C1'	-5.94	118.78	126.50
55	2x	14	A	C5-C6-N1	-5.92	114.74	117.70
1	2A	2155	G	C6-N1-C2	5.91	128.65	125.10
55	1x	46	G	N3-C2-N2	-5.91	115.77	119.90
55	1x	46	G	C5-C6-N1	5.91	114.45	111.50
55	1x	46	G	N9-C4-C5	5.91	107.76	105.40
32	1a	560	U	C2-N1-C1'	5.90	124.78	117.70
1	1A	1170	G	C8-N9-C4	-5.89	104.04	106.40
1	2A	1313	U	C2-N1-C1'	5.88	124.75	117.70
1	1A	845	G	O4'-C1'-N9	5.87	112.90	108.20
32	2a	1027	C	N3-C2-O2	-5.86	117.80	121.90
32	1a	1002	G	C8-N9-C1'	-5.86	119.39	127.00
1	1A	226	G	O4'-C1'-N9	5.86	112.89	108.20
55	1x	46	G	N1-C2-N3	5.85	127.41	123.90
1	2A	2473	U	C2-N1-C1'	5.84	124.71	117.70
1	2A	2897	U	N1-C2-O2	5.83	126.88	122.80
54	1y	33	U	N1-C2-O2	5.82	126.87	122.80
54	1w	1	G	N9-C4-C5	-5.82	103.07	105.40
1	1A	2061	G	O5'-P-OP2	-5.81	100.47	105.70
2	2B	80	U	C5'-C4'-O4'	5.79	116.05	109.10
55	1x	22	G	C5-C6-N1	5.76	114.38	111.50
54	1w	1	G	C8-N9-C1'	-5.75	119.52	127.00
54	2w	76	A	O4'-C1'-N9	5.74	112.80	108.20
32	2a	1039	C	N1-C2-O2	5.74	122.34	118.90
32	2a	1052	U	N1-C2-O2	5.74	126.82	122.80
34	1c	190	ARG	NE-CZ-NH1	-5.74	117.43	120.30
32	2a	65	U	P-O3'-C3'	5.71	126.56	119.70
55	2x	46	G	N3-C2-N2	-5.70	115.91	119.90
32	1a	1030(B)	C	N3-C2-O2	-5.70	117.91	121.90
32	1a	1030(B)	C	C5-C6-N1	5.69	123.84	121.00
1	2A	527	C	C2-N1-C1'	5.68	125.05	118.80
1	2A	1575	C	N1-C2-O2	5.68	122.31	118.90
32	1a	266	G	P-O3'-C3'	5.67	126.51	119.70
32	2a	1206	G	N3-C4-N9	5.63	129.38	126.00
1	2A	2136	C	N3-C2-O2	-5.62	117.97	121.90
1	1A	2032	G	C5-N7-C8	5.61	107.11	104.30
55	1x	22	G	N3-C4-C5	5.55	131.38	128.60
32	2a	1039	C	C5-C4-N4	-5.55	116.32	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1074	G	C4-N9-C1'	5.54	133.70	126.50
55	1x	46	G	C5-C6-O6	-5.54	125.28	128.60
1	1A	1100	C	C6-N1-C1'	-5.53	114.16	120.80
1	1A	1170	G	N7-C8-N9	5.53	115.86	113.10
32	2a	754	C	N1-C2-O2	5.53	122.22	118.90
1	2A	746	A	O4'-C1'-N9	5.53	112.62	108.20
54	1w	1	G	C4-N9-C1'	5.52	133.67	126.50
32	2a	266	G	P-O3'-C3'	5.52	126.32	119.70
1	1A	1177	A	O5'-P-OP1	-5.52	100.74	105.70
1	2A	1992	G	P-O3'-C3'	5.51	126.31	119.70
1	2A	2156	G	C8-N9-C4	-5.51	104.20	106.40
32	2a	266	G	N3-C4-C5	-5.51	125.84	128.60
32	2a	1003	G	C4-N9-C1'	5.51	133.66	126.50
1	2A	787	U	O5'-P-OP1	-5.49	100.76	105.70
32	2a	1040	U	C5-C4-O4	5.48	129.19	125.90
1	1A	975	C	C2-N3-C4	-5.48	117.16	119.90
1	2A	2206	G	C8-N9-C1'	5.48	134.12	127.00
55	1x	14	A	C5-C6-N1	-5.48	114.96	117.70
55	2x	22	G	N1-C6-O6	-5.47	116.62	119.90
1	1A	1372	U	N3-C4-O4	5.46	123.22	119.40
54	2y	22	G	N1-C6-O6	5.45	123.17	119.90
54	1y	58	A	N1-C6-N6	5.44	121.86	118.60
54	1y	33	U	C2-N1-C1'	5.44	124.22	117.70
32	2a	1001(A)	G	N3-C4-C5	-5.42	125.89	128.60
1	1A	2554	U	O5'-P-OP1	-5.42	100.82	105.70
1	2A	1530	C	P-O3'-C3'	5.42	126.20	119.70
1	2A	265	A	O4'-C1'-N9	5.42	112.53	108.20
54	2w	69	G	C5-C6-O6	-5.41	125.35	128.60
1	1A	1313	U	C2-N1-C1'	5.40	124.18	117.70
1	1A	1131	G	O4'-C1'-N9	5.38	112.50	108.20
1	2A	2139	C	N3-C2-O2	-5.37	118.14	121.90
1	1A	889	C	N1-C2-O2	5.36	122.12	118.90
1	2A	1313	U	O4'-C1'-N1	5.36	112.49	108.20
32	2a	998	G	C4-C5-N7	-5.35	108.66	110.80
32	2a	1040	U	O4'-C1'-N1	5.34	112.47	108.20
55	1x	22	G	C4-N9-C1'	-5.34	119.56	126.50
55	1x	46	G	C4-C5-N7	-5.33	108.67	110.80
1	2A	512	G	O4'-C1'-N9	5.33	112.47	108.20
32	1a	1067	A	P-O3'-C3'	5.33	126.09	119.70
55	1x	10	G	N3-C2-N2	-5.33	116.17	119.90
1	2A	2473	U	N1-C2-O2	5.31	126.52	122.80
54	2w	67	C	C2-N3-C4	5.30	122.55	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	2x	22	G	C8-N9-C1'	5.30	133.89	127.00
1	2A	527	C	C6-N1-C1'	-5.30	114.44	120.80
32	2a	1025	U	O4'-C1'-N1	5.28	112.42	108.20
1	1A	748	G	N1-C6-O6	-5.27	116.74	119.90
55	2x	22	G	C4-C5-C6	-5.27	115.64	118.80
1	1A	999	U	O5'-P-OP2	-5.26	100.96	105.70
1	1A	975	C	N3-C2-O2	5.26	125.58	121.90
32	2a	1004	A	N1-C6-N6	-5.26	115.44	118.60
32	2a	1158	C	N1-C2-O2	5.25	122.05	118.90
55	1x	14	A	C4-N9-C1'	5.25	135.75	126.30
54	2w	10	G	N3-C2-N2	-5.25	116.23	119.90
54	2y	62	C	C2-N3-C4	5.24	122.52	119.90
32	1a	1201	A	P-O3'-C3'	5.23	125.98	119.70
40	1i	50	LEU	CA-CB-CG	5.23	127.32	115.30
54	1w	72	C	C5-C6-N1	5.23	123.61	121.00
1	1A	1076	C	O4'-C1'-N1	5.22	112.38	108.20
1	1A	1100	C	N1-C2-O2	5.21	122.02	118.90
55	1x	14	A	C8-N9-C1'	-5.21	118.33	127.70
55	2x	76	A	C4-C5-N7	-5.21	108.10	110.70
1	1A	2028	U	N3-C4-O4	-5.20	115.76	119.40
1	1A	889	C	C2-N1-C1'	5.20	124.52	118.80
1	1A	944	G	C4-N9-C1'	5.20	133.26	126.50
1	2A	845	G	C4-N9-C1'	5.20	133.26	126.50
1	1A	1352	U	O5'-P-OP1	-5.19	101.03	105.70
1	1A	1074	G	C8-N9-C1'	-5.18	120.26	127.00
4	2E	72	VAL	C-N-CA	5.18	134.65	121.70
1	1A	1063	G	N1-C6-O6	-5.18	116.79	119.90
1	1A	1175	U	P-O3'-C3'	5.17	125.91	119.70
54	1w	1	G	C6-C5-N7	-5.17	127.30	130.40
32	1a	1206	G	C5-C6-O6	-5.16	125.50	128.60
32	2a	1206	G	N3-C4-C5	-5.16	126.02	128.60
1	1A	12	U	C6-N1-C1'	-5.15	113.99	121.20
1	1A	1313	U	N3-C2-O2	-5.15	118.59	122.20
32	2a	1039	C	C2-N1-C1'	5.15	124.47	118.80
1	1A	1075	C	C6-N1-C2	-5.15	118.24	120.30
54	1w	72	C	C5-C4-N4	-5.14	116.60	120.20
1	1A	34	C	N1-C2-O2	5.14	121.98	118.90
32	1a	1158	C	C2-N1-C1'	5.14	124.45	118.80
32	2a	687	A	P-O3'-C3'	5.14	125.86	119.70
32	2a	1025	U	C2-N1-C1'	-5.14	111.54	117.70
1	2A	614	U	N3-C2-O2	-5.13	118.61	122.20
32	1a	1043	C	C2-N1-C1'	5.12	124.44	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	277	C	C6-N1-C1'	-5.12	114.65	120.80
32	2a	1027	C	N1-C2-O2	5.11	121.97	118.90
1	2A	1129	A	O4'-C1'-N9	5.11	112.29	108.20
1	2A	1022	G	C6-C5-N7	5.10	133.46	130.40
1	1A	1086	A	C2-N3-C4	5.10	113.15	110.60
32	1a	1002	G	N3-C4-C5	-5.09	126.05	128.60
32	2a	501	C	C6-N1-C2	-5.09	118.26	120.30
1	1A	12	U	N1-C2-O2	5.08	126.36	122.80
1	1A	1617	C	C2-N1-C1'	-5.08	113.22	118.80
54	2y	63	G	C6-N1-C2	5.07	128.14	125.10
1	2A	228	A	P-O3'-C3'	5.07	125.78	119.70
32	1a	1285	A	P-O3'-C3'	5.07	125.78	119.70
32	2a	1206	G	C5-C6-O6	-5.06	125.56	128.60
1	1A	1074	G	N3-C4-N9	5.05	129.03	126.00
34	1c	190	ARG	NE-CZ-NH2	5.04	122.82	120.30
54	1w	75	C	P-O3'-C3'	5.04	125.75	119.70
1	1A	944	G	C8-N9-C1'	-5.03	120.46	127.00
54	2w	75	C	P-O3'-C3'	5.03	125.74	119.70
32	1a	266	G	O4'-C1'-N9	-5.03	104.18	108.20
32	1a	21	G	O5'-P-OP1	-5.03	101.17	105.70
1	2A	1022	G	N3-C2-N2	-5.02	116.39	119.90
1	1A	1075	C	C5-C6-N1	5.01	123.51	121.00
1	1A	1068	G	O4'-C1'-N9	5.01	112.21	108.20
1	1A	1372	U	C5-C4-O4	-5.01	122.89	125.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	14	67	TYR	Peptide
50	2s	28	LYS	Peptide

5.2 Too-close contacts ⓘ

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	259 (95%)	13 (5%)	1 (0%)	34	57
3	2D	273/276 (99%)	261 (96%)	11 (4%)	1 (0%)	34	57
4	1E	202/206 (98%)	194 (96%)	7 (4%)	1 (0%)	29	52
4	2E	202/206 (98%)	194 (96%)	6 (3%)	2 (1%)	15	32
5	1F	201/210 (96%)	195 (97%)	5 (2%)	1 (0%)	29	52
5	2F	201/210 (96%)	195 (97%)	4 (2%)	2 (1%)	15	32
6	1G	179/182 (98%)	167 (93%)	10 (6%)	2 (1%)	14	30
6	2G	179/182 (98%)	165 (92%)	12 (7%)	2 (1%)	14	30
7	1H	172/180 (96%)	162 (94%)	9 (5%)	1 (1%)	25	47
7	2H	172/180 (96%)	160 (93%)	11 (6%)	1 (1%)	25	47
8	1I	144/148 (97%)	126 (88%)	13 (9%)	5 (4%)	3	5
8	2I	144/148 (97%)	129 (90%)	14 (10%)	1 (1%)	22	43
9	1N	138/140 (99%)	130 (94%)	8 (6%)	0	100	100
9	2N	138/140 (99%)	128 (93%)	10 (7%)	0	100	100
10	1O	120/122 (98%)	112 (93%)	7 (6%)	1 (1%)	19	39
10	2O	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
11	1P	147/150 (98%)	139 (95%)	7 (5%)	1 (1%)	22	43
11	2P	147/150 (98%)	135 (92%)	10 (7%)	2 (1%)	11	22
12	1Q	139/141 (99%)	130 (94%)	9 (6%)	0	100	100
12	2Q	139/141 (99%)	131 (94%)	7 (5%)	1 (1%)	22	43
13	1R	116/118 (98%)	109 (94%)	7 (6%)	0	100	100
13	2R	116/118 (98%)	109 (94%)	7 (6%)	0	100	100
14	1S	108/112 (96%)	106 (98%)	2 (2%)	0	100	100
14	2S	108/112 (96%)	104 (96%)	3 (3%)	1 (1%)	17	35
15	1T	129/146 (88%)	119 (92%)	9 (7%)	1 (1%)	19	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	2T	129/146 (88%)	121 (94%)	8 (6%)	0	100	100
16	1U	114/118 (97%)	114 (100%)	0	0	100	100
16	2U	114/118 (97%)	114 (100%)	0	0	100	100
17	1V	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	15	32
17	2V	99/101 (98%)	96 (97%)	2 (2%)	1 (1%)	15	32
18	1W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
18	2W	110/113 (97%)	110 (100%)	0	0	100	100
19	1X	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
19	2X	93/96 (97%)	88 (95%)	4 (4%)	1 (1%)	14	30
20	1Y	105/110 (96%)	97 (92%)	6 (6%)	2 (2%)	8	15
20	2Y	105/110 (96%)	99 (94%)	5 (5%)	1 (1%)	15	32
21	1Z	148/206 (72%)	128 (86%)	16 (11%)	4 (3%)	5	8
21	2Z	156/206 (76%)	131 (84%)	22 (14%)	3 (2%)	8	15
22	10	81/85 (95%)	78 (96%)	3 (4%)	0	100	100
22	20	81/85 (95%)	76 (94%)	3 (4%)	2 (2%)	5	9
23	11	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	14	30
23	21	95/98 (97%)	91 (96%)	3 (3%)	1 (1%)	14	30
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
25	13	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
25	23	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
26	14	67/71 (94%)	53 (79%)	8 (12%)	6 (9%)	1	0
26	24	67/71 (94%)	52 (78%)	8 (12%)	7 (10%)	0	0
27	15	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	25	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
28	16	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
28	26	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
29	17	46/49 (94%)	44 (96%)	2 (4%)	0	100	100
29	27	46/49 (94%)	44 (96%)	1 (2%)	1 (2%)	6	12
30	18	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
30	28	62/65 (95%)	60 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	35 (100%)	0	0	100	100
33	1b	229/256 (90%)	197 (86%)	27 (12%)	5 (2%)	6	12
33	2b	229/256 (90%)	199 (87%)	21 (9%)	9 (4%)	3	4
34	1c	204/239 (85%)	183 (90%)	19 (9%)	2 (1%)	15	32
34	2c	204/239 (85%)	181 (89%)	20 (10%)	3 (2%)	10	21
35	1d	206/209 (99%)	191 (93%)	15 (7%)	0	100	100
35	2d	206/209 (99%)	191 (93%)	15 (7%)	0	100	100
36	1e	146/162 (90%)	142 (97%)	2 (1%)	2 (1%)	11	22
36	2e	146/162 (90%)	141 (97%)	5 (3%)	0	100	100
37	1f	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
37	2f	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
38	1g	153/156 (98%)	142 (93%)	9 (6%)	2 (1%)	12	24
38	2g	153/156 (98%)	140 (92%)	11 (7%)	2 (1%)	12	24
39	1h	135/138 (98%)	131 (97%)	4 (3%)	0	100	100
39	2h	135/138 (98%)	128 (95%)	6 (4%)	1 (1%)	22	43
40	1i	125/128 (98%)	108 (86%)	17 (14%)	0	100	100
40	2i	125/128 (98%)	107 (86%)	17 (14%)	1 (1%)	19	39
41	1j	95/105 (90%)	81 (85%)	8 (8%)	6 (6%)	1	1
41	2j	94/105 (90%)	80 (85%)	9 (10%)	5 (5%)	2	2
42	1k	112/129 (87%)	105 (94%)	7 (6%)	0	100	100
42	2k	112/129 (87%)	105 (94%)	7 (6%)	0	100	100
43	1l	119/132 (90%)	113 (95%)	6 (5%)	0	100	100
43	2l	119/132 (90%)	112 (94%)	7 (6%)	0	100	100
44	1m	121/126 (96%)	113 (93%)	6 (5%)	2 (2%)	9	18
44	2m	120/126 (95%)	110 (92%)	7 (6%)	3 (2%)	5	9
45	1n	58/61 (95%)	54 (93%)	4 (7%)	0	100	100
45	2n	58/61 (95%)	54 (93%)	4 (7%)	0	100	100
46	1o	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
46	2o	86/89 (97%)	80 (93%)	4 (5%)	2 (2%)	6	11
47	1p	80/88 (91%)	75 (94%)	4 (5%)	1 (1%)	12	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	2p	80/88 (91%)	74 (92%)	5 (6%)	1 (1%)	12	24
48	1q	97/105 (92%)	90 (93%)	6 (6%)	1 (1%)	15	32
48	2q	97/105 (92%)	91 (94%)	6 (6%)	0	100	100
49	1r	66/88 (75%)	63 (96%)	3 (4%)	0	100	100
49	2r	66/88 (75%)	64 (97%)	2 (3%)	0	100	100
50	1s	81/93 (87%)	73 (90%)	6 (7%)	2 (2%)	5	9
50	2s	81/93 (87%)	72 (89%)	7 (9%)	2 (2%)	5	9
51	1t	94/106 (89%)	87 (93%)	2 (2%)	5 (5%)	2	2
51	2t	94/106 (89%)	87 (93%)	1 (1%)	6 (6%)	1	1
52	1u	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
52	2u	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
All	All	11370/12128 (94%)	10613 (93%)	636 (6%)	121 (1%)	14	30

All (121) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	1D	275	LYS
5	1F	130	ALA
6	1G	47	LYS
6	1G	51	ARG
7	1H	126	PRO
17	1V	79	VAL
21	1Z	159	PRO
23	11	3	LYS
26	14	53	GLU
33	1b	17	PHE
38	1g	79	ARG
38	1g	80	VAL
41	1j	55	LYS
44	1m	3	ARG
47	1p	53	VAL
48	1q	68	ARG
51	1t	95	ALA
3	2D	3	VAL
5	2F	21	ALA
5	2F	130	ALA
7	2H	126	PRO
8	2I	10	GLU

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Mol	Chain	Res	Type
12	2Q	28	ALA
17	2V	79	VAL
26	24	53	GLU
26	24	55	ARG
29	27	46	VAL
33	2b	16	HIS
33	2b	17	PHE
33	2b	123	ALA
33	2b	126	GLU
41	2j	29	ARG
47	2p	53	VAL
51	2t	95	ALA
8	1I	106	GLY
26	14	45	GLY
26	14	47	GLN
26	14	56	VAL
33	1b	165	VAL
34	1c	66	VAL
41	1j	29	ARG
41	1j	75	ILE
50	1s	42	PRO
51	1t	47	GLY
14	2S	84	GLN
22	20	4	LYS
22	20	13	GLY
26	24	45	GLY
26	24	48	ARG
26	24	62	ARG
33	2b	165	VAL
34	2c	107	GLN
38	2g	80	VAL
41	2j	75	ILE
44	2m	4	ILE
50	2s	29	ARG
50	2s	42	PRO
51	2t	10	LEU
51	2t	47	GLY
4	1E	52	LEU
8	1I	10	GLU
8	1I	105	HIS
21	1Z	134	PRO
21	1Z	152	ALA

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Mol	Chain	Res	Type
33	1b	10	LEU
33	1b	231	GLU
36	1e	86	ALA
41	1j	78	ASN
51	1t	100	ILE
6	2G	48	GLU
6	2G	51	ARG
23	2l	3	LYS
33	2b	125	PRO
33	2b	231	GLU
38	2g	7	ALA
40	2i	54	ASP
41	2j	55	LYS
41	2j	78	ASN
51	2t	102	GLY
8	1I	107	VAL
26	14	44	THR
36	1e	85	GLY
41	1j	77	PRO
44	1m	67	GLU
4	2E	52	LEU
4	2E	73	GLU
11	2P	38	GLN
19	2X	2	LYS
21	2Z	134	PRO
21	2Z	171	ILE
26	24	46	GLN
26	24	49	PHE
34	2c	3	ASN
34	2c	108	ASN
44	2m	67	GLU
51	2t	9	ASN
15	1T	128	GLU
20	1Y	54	LYS
26	14	62	ARG
34	1c	3	ASN
11	2P	45	LEU
39	2h	73	ASP
41	2j	77	PRO
46	2o	88	ARG
8	1I	11	ASN
10	1O	29	ASN

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Mol	Chain	Res	Type
21	1Z	163	LEU
50	1s	81	ARG
51	1t	10	LEU
33	2b	10	LEU
46	2o	23	GLY
51	2t	100	ILE
44	2m	6	GLY
33	1b	124	SER
11	1P	122	PRO
51	1t	102	GLY
21	2Z	146	ILE
20	1Y	103	GLY
41	1j	91	PRO
20	2Y	103	GLY
33	2b	234	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	215/218 (99%)	208 (97%)	7 (3%)	38	64
3	2D	215/218 (99%)	207 (96%)	8 (4%)	34	60
4	1E	164/166 (99%)	154 (94%)	10 (6%)	18	38
4	2E	164/166 (99%)	151 (92%)	13 (8%)	12	24
5	1F	160/166 (96%)	149 (93%)	11 (7%)	15	31
5	2F	159/166 (96%)	149 (94%)	10 (6%)	18	36
6	1G	144/156 (92%)	136 (94%)	8 (6%)	21	42
6	2G	143/156 (92%)	135 (94%)	8 (6%)	21	42
7	1H	144/148 (97%)	140 (97%)	4 (3%)	43	69
7	2H	144/148 (97%)	140 (97%)	4 (3%)	43	69
8	1I	113/124 (91%)	110 (97%)	3 (3%)	44	71
8	2I	105/124 (85%)	102 (97%)	3 (3%)	42	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	1N	118/119 (99%)	114 (97%)	4 (3%)	37	63
9	2N	118/119 (99%)	115 (98%)	3 (2%)	47	73
10	1O	100/100 (100%)	98 (98%)	2 (2%)	55	78
10	2O	100/100 (100%)	99 (99%)	1 (1%)	76	90
11	1P	115/116 (99%)	110 (96%)	5 (4%)	29	54
11	2P	115/116 (99%)	113 (98%)	2 (2%)	60	81
12	1Q	111/111 (100%)	110 (99%)	1 (1%)	78	91
12	2Q	111/111 (100%)	109 (98%)	2 (2%)	59	80
13	1R	101/101 (100%)	90 (89%)	11 (11%)	6	11
13	2R	101/101 (100%)	92 (91%)	9 (9%)	9	19
14	1S	86/88 (98%)	84 (98%)	2 (2%)	50	75
14	2S	85/88 (97%)	82 (96%)	3 (4%)	36	62
15	1T	115/127 (91%)	113 (98%)	2 (2%)	60	81
15	2T	113/127 (89%)	112 (99%)	1 (1%)	78	91
16	1U	93/94 (99%)	90 (97%)	3 (3%)	39	65
16	2U	93/94 (99%)	92 (99%)	1 (1%)	73	88
17	1V	80/82 (98%)	73 (91%)	7 (9%)	10	19
17	2V	80/82 (98%)	76 (95%)	4 (5%)	24	47
18	1W	90/92 (98%)	86 (96%)	4 (4%)	28	53
18	2W	90/92 (98%)	87 (97%)	3 (3%)	38	64
19	1X	77/78 (99%)	75 (97%)	2 (3%)	46	72
19	2X	77/78 (99%)	75 (97%)	2 (3%)	46	72
20	1Y	85/91 (93%)	81 (95%)	4 (5%)	26	50
20	2Y	85/91 (93%)	84 (99%)	1 (1%)	71	87
21	1Z	135/179 (75%)	131 (97%)	4 (3%)	41	67
21	2Z	137/179 (76%)	134 (98%)	3 (2%)	52	76
22	10	65/67 (97%)	64 (98%)	1 (2%)	65	83
22	20	65/67 (97%)	65 (100%)	0	100	100
23	11	80/83 (96%)	79 (99%)	1 (1%)	69	86
23	21	80/83 (96%)	80 (100%)	0	100	100
24	12	65/67 (97%)	64 (98%)	1 (2%)	65	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	22	65/67 (97%)	63 (97%)	2 (3%)	40	66
25	13	51/52 (98%)	49 (96%)	2 (4%)	32	58
25	23	50/52 (96%)	48 (96%)	2 (4%)	31	57
26	14	59/63 (94%)	53 (90%)	6 (10%)	7	14
26	24	53/63 (84%)	49 (92%)	4 (8%)	13	27
27	15	50/52 (96%)	46 (92%)	4 (8%)	12	24
27	25	50/52 (96%)	47 (94%)	3 (6%)	19	39
28	16	51/52 (98%)	49 (96%)	2 (4%)	32	58
28	26	50/52 (96%)	47 (94%)	3 (6%)	19	39
29	17	41/42 (98%)	40 (98%)	1 (2%)	49	74
29	27	41/42 (98%)	40 (98%)	1 (2%)	49	74
30	18	54/55 (98%)	52 (96%)	2 (4%)	34	60
30	28	54/55 (98%)	52 (96%)	2 (4%)	34	60
31	19	34/34 (100%)	34 (100%)	0	100	100
31	29	34/34 (100%)	32 (94%)	2 (6%)	19	39
33	1b	192/220 (87%)	186 (97%)	6 (3%)	40	66
33	2b	187/220 (85%)	183 (98%)	4 (2%)	53	77
34	1c	142/188 (76%)	139 (98%)	3 (2%)	53	77
34	2c	140/188 (74%)	139 (99%)	1 (1%)	84	94
35	1d	169/181 (93%)	164 (97%)	5 (3%)	41	67
35	2d	173/181 (96%)	170 (98%)	3 (2%)	60	81
36	1e	113/123 (92%)	110 (97%)	3 (3%)	44	71
36	2e	114/123 (93%)	112 (98%)	2 (2%)	59	80
37	1f	84/90 (93%)	84 (100%)	0	100	100
37	2f	85/90 (94%)	85 (100%)	0	100	100
38	1g	119/127 (94%)	119 (100%)	0	100	100
38	2g	120/127 (94%)	117 (98%)	3 (2%)	47	73
39	1h	114/119 (96%)	112 (98%)	2 (2%)	59	80
39	2h	114/119 (96%)	113 (99%)	1 (1%)	78	91
40	1i	90/99 (91%)	86 (96%)	4 (4%)	28	53
40	2i	89/99 (90%)	85 (96%)	4 (4%)	27	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	1j	66/92 (72%)	65 (98%)	1 (2%)	65	83
41	2j	69/92 (75%)	68 (99%)	1 (1%)	67	85
42	1k	82/99 (83%)	80 (98%)	2 (2%)	49	74
42	2k	83/99 (84%)	82 (99%)	1 (1%)	71	87
43	1l	96/108 (89%)	92 (96%)	4 (4%)	30	55
43	2l	96/108 (89%)	94 (98%)	2 (2%)	53	77
44	1m	93/101 (92%)	91 (98%)	2 (2%)	52	76
44	2m	92/101 (91%)	90 (98%)	2 (2%)	52	76
45	1n	49/50 (98%)	45 (92%)	4 (8%)	11	22
45	2n	49/50 (98%)	45 (92%)	4 (8%)	11	22
46	1o	78/80 (98%)	78 (100%)	0	100	100
46	2o	78/80 (98%)	75 (96%)	3 (4%)	33	59
47	1p	69/74 (93%)	65 (94%)	4 (6%)	20	40
47	2p	68/74 (92%)	64 (94%)	4 (6%)	19	39
48	1q	94/97 (97%)	93 (99%)	1 (1%)	73	88
48	2q	94/97 (97%)	92 (98%)	2 (2%)	53	77
49	1r	59/77 (77%)	56 (95%)	3 (5%)	24	46
49	2r	59/77 (77%)	55 (93%)	4 (7%)	16	32
50	1s	69/80 (86%)	69 (100%)	0	100	100
50	2s	67/80 (84%)	67 (100%)	0	100	100
51	1t	70/82 (85%)	67 (96%)	3 (4%)	29	54
51	2t	70/82 (85%)	68 (97%)	2 (3%)	42	68
52	1u	18/22 (82%)	18 (100%)	0	100	100
52	2u	18/22 (82%)	18 (100%)	0	100	100
All	All	9304/10064 (92%)	9000 (97%)	304 (3%)	38	64

All (304) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	94	LEU
3	1D	142	VAL
3	1D	193	VAL
3	1D	211	ARG
3	1D	229	VAL

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Mol	Chain	Res	Type
3	1D	242	ARG
3	1D	257	LEU
4	1E	9	VAL
4	1E	21	VAL
4	1E	24	THR
4	1E	77	ILE
4	1E	116	VAL
4	1E	144	ARG
4	1E	170	LEU
4	1E	181	LEU
4	1E	184	VAL
4	1E	195	LEU
5	1F	28	ILE
5	1F	33	LEU
5	1F	53	THR
5	1F	106	ARG
5	1F	125	LEU
5	1F	132	VAL
5	1F	158	THR
5	1F	170	LEU
5	1F	183	VAL
5	1F	192	LEU
5	1F	201	VAL
6	1G	3	LEU
6	1G	5	VAL
6	1G	7	LEU
6	1G	43	LEU
6	1G	82	LEU
6	1G	109	VAL
6	1G	150	ASP
6	1G	159	VAL
7	1H	15	VAL
7	1H	84	SER
7	1H	129	THR
7	1H	152	ARG
8	1I	47	LEU
8	1I	57	ARG
8	1I	92	VAL
9	1N	33	LEU
9	1N	34	LEU
9	1N	35	ARG
9	1N	48	MET

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Mol	Chain	Res	Type
10	1O	10	VAL
10	1O	24	VAL
11	1P	65	ARG
11	1P	83	VAL
11	1P	95	VAL
11	1P	106	LEU
11	1P	147	LEU
12	1Q	109	VAL
13	1R	18	LEU
13	1R	24	GLN
13	1R	28	LEU
13	1R	29	LEU
13	1R	33	ARG
13	1R	36	THR
13	1R	44	LEU
13	1R	54	LEU
13	1R	65	LEU
13	1R	100	LEU
13	1R	111	LEU
14	1S	14	VAL
14	1S	52	SER
15	1T	28	VAL
15	1T	89	VAL
16	1U	8	VAL
16	1U	31	SER
16	1U	95	LEU
17	1V	18	LEU
17	1V	46	VAL
17	1V	51	VAL
17	1V	61	VAL
17	1V	72	VAL
17	1V	79	VAL
17	1V	82	ARG
18	1W	1	MET
18	1W	23	LEU
18	1W	67	ASP
18	1W	107	LEU
19	1X	35	THR
19	1X	76	ARG
20	1Y	1	MET
20	1Y	43	ASN
20	1Y	72	VAL

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Mol	Chain	Res	Type
20	1Y	97	ARG
21	1Z	86	VAL
21	1Z	91	LEU
21	1Z	154	ASP
21	1Z	171	ILE
22	10	7	LEU
23	11	59	THR
24	12	19	VAL
25	13	8	LEU
25	13	54	VAL
26	14	34	GLU
26	14	49	PHE
26	14	50	VAL
26	14	56	VAL
26	14	58	ARG
26	14	63	TYR
27	15	6	VAL
27	15	16	ARG
27	15	29	THR
27	15	33	CYS
28	16	6	ARG
28	16	48	VAL
29	17	24	THR
30	18	31	HIS
30	18	32	LEU
33	1b	8	LYS
33	1b	21	ARG
33	1b	24	TRP
33	1b	35	GLU
33	1b	189	ASP
33	1b	196	LEU
34	1c	28	GLN
34	1c	70	VAL
34	1c	115	LEU
35	1d	31	CYS
35	1d	115	ARG
35	1d	135	LEU
35	1d	158	ILE
35	1d	200	GLU
36	1e	12	LEU
36	1e	31	LEU
36	1e	41	VAL

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Mol	Chain	Res	Type
39	1h	51	VAL
39	1h	112	LEU
40	1i	42	ARG
40	1i	50	LEU
40	1i	65	VAL
40	1i	108	VAL
41	1j	92	THR
42	1k	31	THR
42	1k	114	VAL
43	1l	27	LEU
43	1l	83	VAL
43	1l	84	LEU
43	1l	123	LYS
44	1m	4	ILE
44	1m	109	THR
45	1n	3	ARG
45	1n	6	LEU
45	1n	18	VAL
45	1n	22	THR
47	1p	2	VAL
47	1p	20	VAL
47	1p	54	GLU
47	1p	67	THR
48	1q	78	GLU
49	1r	26	LEU
49	1r	31	LEU
49	1r	47	THR
51	1t	10	LEU
51	1t	13	LEU
51	1t	62	LEU
3	2D	3	VAL
3	2D	94	LEU
3	2D	103	ARG
3	2D	142	VAL
3	2D	193	VAL
3	2D	211	ARG
3	2D	229	VAL
3	2D	242	ARG
4	2E	9	VAL
4	2E	12	THR
4	2E	21	VAL
4	2E	47	VAL

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Mol	Chain	Res	Type
4	2E	52	LEU
4	2E	75	VAL
4	2E	116	VAL
4	2E	144	ARG
4	2E	170	LEU
4	2E	175	VAL
4	2E	181	LEU
4	2E	184	VAL
4	2E	195	LEU
5	2F	33	LEU
5	2F	53	THR
5	2F	70	THR
5	2F	88	VAL
5	2F	93	LYS
5	2F	106	ARG
5	2F	158	THR
5	2F	170	LEU
5	2F	183	VAL
5	2F	192	LEU
6	2G	3	LEU
6	2G	21	ARG
6	2G	43	LEU
6	2G	49	ASP
6	2G	60	LEU
6	2G	79	ASN
6	2G	140	ILE
6	2G	159	VAL
7	2H	63	SER
7	2H	125	VAL
7	2H	136	ILE
7	2H	152	ARG
8	2I	20	ASP
8	2I	47	LEU
8	2I	92	VAL
9	2N	32	THR
9	2N	33	LEU
9	2N	34	LEU
10	2O	24	VAL
11	2P	95	VAL
11	2P	147	LEU
12	2Q	1	MET
12	2Q	109	VAL

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Mol	Chain	Res	Type
13	2R	18	LEU
13	2R	24	GLN
13	2R	29	LEU
13	2R	33	ARG
13	2R	44	LEU
13	2R	60	LEU
13	2R	65	LEU
13	2R	79	LEU
13	2R	100	LEU
14	2S	8	GLU
14	2S	14	VAL
14	2S	52	SER
15	2T	89	VAL
16	2U	31	SER
17	2V	18	LEU
17	2V	46	VAL
17	2V	72	VAL
17	2V	79	VAL
18	2W	1	MET
18	2W	67	ASP
18	2W	107	LEU
19	2X	35	THR
19	2X	65	ARG
20	2Y	43	ASN
21	2Z	142	SER
21	2Z	154	ASP
21	2Z	161	VAL
24	22	52	ASP
24	22	66	GLU
25	23	8	LEU
25	23	30	ARG
26	24	34	GLU
26	24	48	ARG
26	24	50	VAL
26	24	56	VAL
27	25	6	VAL
27	25	16	ARG
27	25	35	GLU
28	26	6	ARG
28	26	48	VAL
28	26	52	VAL
29	27	1	MET

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Mol	Chain	Res	Type
30	28	31	HIS
30	28	32	LEU
31	29	4	ARG
31	29	7	VAL
33	2b	35	GLU
33	2b	128	GLU
33	2b	189	ASP
33	2b	215	LEU
34	2c	70	VAL
35	2d	135	LEU
35	2d	170	VAL
35	2d	194	LEU
36	2e	12	LEU
36	2e	41	VAL
38	2g	72	ARG
38	2g	79	ARG
38	2g	104	LEU
39	2h	51	VAL
40	2i	50	LEU
40	2i	65	VAL
40	2i	89	ASN
40	2i	102	LEU
41	2j	89	ASP
42	2k	114	VAL
43	2l	27	LEU
43	2l	84	LEU
44	2m	47	ASP
44	2m	117	VAL
45	2n	3	ARG
45	2n	6	LEU
45	2n	18	VAL
45	2n	22	THR
46	2o	7	GLU
46	2o	21	ASP
46	2o	39	LEU
47	2p	2	VAL
47	2p	5	ARG
47	2p	20	VAL
47	2p	62	VAL
48	2q	9	VAL
48	2q	63	ARG
49	2r	26	LEU

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Mol	Chain	Res	Type
49	2r	47	THR
49	2r	76	LEU
49	2r	85	LEU
51	2t	62	LEU
51	2t	89	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (100) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	87	ASN
3	1D	126	GLN
4	1E	48	GLN
5	1F	8	GLN
5	1F	69	HIS
6	1G	41	GLN
8	1I	104	GLN
15	1T	58	ASN
15	1T	123	GLN
16	1U	81	HIS
19	1X	31	HIS
19	1X	82	GLN
20	1Y	43	ASN
21	1Z	73	GLN
22	10	3	HIS
24	12	9	GLN
24	12	65	ASN
25	13	32	GLN
33	1b	40	HIS
34	1c	6	HIS
34	1c	37	GLN
34	1c	162	GLN
35	1d	42	GLN
35	1d	77	ASN
35	1d	116	GLN
35	1d	123	HIS
35	1d	161	ASN
37	1f	100	ASN
38	1g	28	ASN
38	1g	86	GLN
40	1i	3	GLN
40	1i	31	GLN
40	1i	34	ASN

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Mol	Chain	Res	Type
40	1i	58	HIS
40	1i	89	ASN
41	1j	56	HIS
43	1l	99	HIS
45	1n	49	HIS
47	1p	13	HIS
50	1s	23	ASN
50	1s	47	HIS
50	1s	69	HIS
50	1s	83	HIS
51	1t	75	ASN
3	2D	87	ASN
3	2D	116	GLN
4	2E	48	GLN
5	2F	69	HIS
6	2G	26	GLN
8	2I	104	GLN
9	2N	38	HIS
9	2N	131	GLN
9	2N	133	GLN
10	2O	3	GLN
12	2Q	12	GLN
12	2Q	13	GLN
14	2S	38	GLN
14	2S	68	GLN
15	2T	58	ASN
15	2T	123	GLN
16	2U	81	HIS
17	2V	64	HIS
18	2W	60	ASN
19	2X	31	HIS
19	2X	82	GLN
20	2Y	43	ASN
21	2Z	55	HIS
21	2Z	73	GLN
21	2Z	132	ASN
23	21	56	GLN
24	22	65	ASN
26	24	46	GLN
31	29	20	HIS
33	2b	40	HIS
33	2b	95	GLN

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Mol	Chain	Res	Type
34	2c	6	HIS
34	2c	37	GLN
34	2c	139	GLN
34	2c	162	GLN
35	2d	42	GLN
35	2d	77	ASN
35	2d	116	GLN
35	2d	123	HIS
35	2d	125	HIS
35	2d	161	ASN
36	2e	20	GLN
36	2e	78	HIS
37	2f	13	ASN
37	2f	100	ASN
38	2g	28	ASN
39	2h	78	GLN
40	2i	3	GLN
40	2i	31	GLN
40	2i	58	HIS
40	2i	89	ASN
42	2k	22	HIS
46	2o	28	GLN
47	2p	13	HIS
50	2s	83	HIS
51	2t	42	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2861/2915 (98%)	440 (15%)	33 (1%)
1	2A	2788/2915 (95%)	516 (18%)	30 (1%)
2	1B	120/121 (99%)	8 (6%)	1 (0%)
2	2B	118/121 (97%)	36 (30%)	0
32	1a	1494/1521 (98%)	226 (15%)	0
32	2a	1498/1521 (98%)	240 (16%)	0
53	1v	12/27 (44%)	3 (25%)	0
53	2v	12/27 (44%)	3 (25%)	0
54	1w	70/76 (92%)	18 (25%)	0
54	1y	71/76 (93%)	23 (32%)	0
54	2w	69/76 (90%)	20 (28%)	0
54	2y	69/76 (90%)	17 (24%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
55	1x	75/77 (97%)	10 (13%)	0
55	2x	75/77 (97%)	9 (12%)	0
All	All	9332/9626 (96%)	1569 (16%)	64 (0%)

All (1569) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	10	G
1	1A	12	U
1	1A	13	A
1	1A	34	C
1	1A	45	C
1	1A	55	G
1	1A	58	G
1	1A	71	A
1	1A	74	A
1	1A	75	G
1	1A	83	G
1	1A	84	A
1	1A	95	G
1	1A	118	A
1	1A	119	A
1	1A	120	U
1	1A	182	A
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	223	A
1	1A	229	A
1	1A	232	G
1	1A	233	A
1	1A	248	G
1	1A	250	G
1	1A	267	C
1	1A	269	U
1	1A	271(E)	U
1	1A	271(L)	U
1	1A	271(M)	G

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Mol	Chain	Res	Type
1	1A	271(S)	G
1	1A	272(B)	G
1	1A	272(J)	C
1	1A	275	G
1	1A	279	C
1	1A	282	A
1	1A	311	A
1	1A	329	G
1	1A	330	A
1	1A	352	G
1	1A	360	G
1	1A	362	U
1	1A	363	G
1	1A	363(B)	G
1	1A	370	G
1	1A	372	G
1	1A	380	U
1	1A	386	G
1	1A	390	A
1	1A	396	G
1	1A	405	U
1	1A	411	G
1	1A	428	A
1	1A	444	C
1	1A	448	U
1	1A	451	C
1	1A	455	C
1	1A	456	C
1	1A	457	A
1	1A	481	G
1	1A	504	U
1	1A	505	A
1	1A	508	G
1	1A	509	C
1	1A	512	G
1	1A	530	G
1	1A	531	C
1	1A	532	A
1	1A	533	G
1	1A	545	G
1	1A	549	G
1	1A	563	G

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Mol	Chain	Res	Type
1	1A	573	G
1	1A	575	A
1	1A	586	A
1	1A	603	A
1	1A	604	G
1	1A	607	U
1	1A	614(B)	G
1	1A	615	G
1	1A	616	G
1	1A	627	A
1	1A	637	A
1	1A	645	C
1	1A	646	A
1	1A	669	G
1	1A	686	G
1	1A	717	G
1	1A	730	C
1	1A	764	A
1	1A	776	G
1	1A	782	A
1	1A	784	A
1	1A	785	G
1	1A	792	G
1	1A	805	G
1	1A	812	C
1	1A	819	A
1	1A	827	U
1	1A	828	U
1	1A	830	G
1	1A	859	G
1	1A	866	A
1	1A	879	G
1	1A	880	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	892	G
1	1A	895	U

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Mol	Chain	Res	Type
1	1A	896	A
1	1A	897	C
1	1A	899	A
1	1A	907	U
1	1A	910	A
1	1A	932	G
1	1A	938	G
1	1A	941	A
1	1A	945	A
1	1A	946	G
1	1A	953	A
1	1A	959	A
1	1A	961	C
1	1A	974	G
1	1A	975	C
1	1A	983	A
1	1A	996	A
1	1A	1005	C
1	1A	1008	C
1	1A	1012	U
1	1A	1013	C
1	1A	1022	G
1	1A	1026	U
1	1A	1033	U
1	1A	1041	C
1	1A	1045	A
1	1A	1046	A
1	1A	1047	G
1	1A	1048	A
1	1A	1051	G
1	1A	1054	A
1	1A	1055	G
1	1A	1058	G
1	1A	1067	A
1	1A	1068	G
1	1A	1071	G
1	1A	1073	A
1	1A	1074	G
1	1A	1075	C
1	1A	1076	C
1	1A	1077	A
1	1A	1078	U

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Mol	Chain	Res	Type
1	1A	1079	C
1	1A	1080	C
1	1A	1085	A
1	1A	1086	A
1	1A	1088	A
1	1A	1089	G
1	1A	1090	U
1	1A	1091	G
1	1A	1094	U
1	1A	1097	U
1	1A	1098	A
1	1A	1100	C
1	1A	1101	U
1	1A	1105	U
1	1A	1107	G
1	1A	1108	U
1	1A	1109	C
1	1A	1110	G
1	1A	1111	A
1	1A	1112	G
1	1A	1116	C
1	1A	1128	A
1	1A	1129	A
1	1A	1130	U
1	1A	1135	C
1	1A	1136	G
1	1A	1149	G
1	1A	1155	A
1	1A	1170	G
1	1A	1171	G
1	1A	1173	G
1	1A	1174	A
1	1A	1175	U
1	1A	1176	G
1	1A	1177	A
1	1A	1210	A
1	1A	1211	U
1	1A	1220	A
1	1A	1241	A
1	1A	1244	G
1	1A	1253	A
1	1A	1256	G

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Mol	Chain	Res	Type
1	1A	1271	G
1	1A	1272	A
1	1A	1273	U
1	1A	1276	A
1	1A	1300	U
1	1A	1301	A
1	1A	1303	G
1	1A	1306	C
1	1A	1313	U
1	1A	1318	C
1	1A	1320	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	1403	C
1	1A	1416	G
1	1A	1417	C
1	1A	1420	U
1	1A	1421	G
1	1A	1428	C
1	1A	1445	A
1	1A	1450	G
1	1A	1455	G
1	1A	1461	G
1	1A	1467	C
1	1A	1471	A
1	1A	1482	G
1	1A	1484	G
1	1A	1493	C
1	1A	1508	A
1	1A	1509	C
1	1A	1509(A)	A
1	1A	1509(B)	A
1	1A	1513	C
1	1A	1514	U
1	1A	1531	C

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Mol	Chain	Res	Type
1	1A	1554	A
1	1A	1558	A
1	1A	1566	A
1	1A	1569	A
1	1A	1578	U
1	1A	1580	A
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	1646	C
1	1A	1647	G
1	1A	1648	C
1	1A	1654	A
1	1A	1674	G
1	1A	1696	G
1	1A	1700	A
1	1A	1701	A
1	1A	1703	G
1	1A	1722	A
1	1A	1739	U
1	1A	1746	G
1	1A	1756	G
1	1A	1762	A
1	1A	1763	G
1	1A	1764	G
1	1A	1773	A
1	1A	1780	A
1	1A	1782	C
1	1A	1791	A
1	1A	1800	C
1	1A	1801	G
1	1A	1816	G
1	1A	1817	G
1	1A	1828	G
1	1A	1829	A
1	1A	1847	A
1	1A	1861	G
1	1A	1877	A
1	1A	1878	G

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Mol	Chain	Res	Type
1	1A	1900	A
1	1A	1906	G
1	1A	1929	G
1	1A	1930	G
1	1A	1937	A
1	1A	1938	A
1	1A	1955	U
1	1A	1963	U
1	1A	1967	C
1	1A	1970	A
1	1A	1971	A
1	1A	1972	A
1	1A	1993	U
1	1A	1997	G
1	1A	2023	G
1	1A	2031	A
1	1A	2032	G
1	1A	2033	A
1	1A	2043	C
1	1A	2055	C
1	1A	2056	G
1	1A	2060	A
1	1A	2061	G
1	1A	2069	G
1	1A	2093	G
1	1A	2096	U
1	1A	2098	U
1	1A	2101	G
1	1A	2110	G
1	1A	2113	U
1	1A	2116	G
1	1A	2119	A
1	1A	2121	G
1	1A	2122	U
1	1A	2126	A
1	1A	2127	G
1	1A	2131	G
1	1A	2132	U
1	1A	2133	G
1	1A	2134	A
1	1A	2135	A
1	1A	2139	C

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Mol	Chain	Res	Type
1	1A	2140	C
1	1A	2142	C
1	1A	2146	C
1	1A	2147	G
1	1A	2151	G
1	1A	2156	G
1	1A	2157	G
1	1A	2159	G
1	1A	2165	G
1	1A	2166	G
1	1A	2171	A
1	1A	2172	U
1	1A	2173	A
1	1A	2178	C
1	1A	2181	G
1	1A	2182	G
1	1A	2184	G
1	1A	2188	C
1	1A	2192	G
1	1A	2198	A
1	1A	2206	G
1	1A	2207	G
1	1A	2225	A
1	1A	2238	G
1	1A	2239	G
1	1A	2268	A
1	1A	2269	A
1	1A	2273	A
1	1A	2283	C
1	1A	2287	A
1	1A	2289	G
1	1A	2305	A
1	1A	2307	G
1	1A	2308	G
1	1A	2314	C
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

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Mol	Chain	Res	Type
1	1A	2372	G
1	1A	2383	G
1	1A	2385	C
1	1A	2406	U
1	1A	2410	G
1	1A	2414	G
1	1A	2425	A
1	1A	2429	G
1	1A	2430	A
1	1A	2435	A
1	1A	2439	A
1	1A	2441	C
1	1A	2448	A
1	1A	2468	G
1	1A	2476	A
1	1A	2487	G
1	1A	2491	U
1	1A	2498	C
1	1A	2502	G
1	1A	2505	G
1	1A	2506	U
1	1A	2518	A
1	1A	2529	G
1	1A	2554	U
1	1A	2566	A
1	1A	2567	G
1	1A	2572	A
1	1A	2573	C
1	1A	2602	A
1	1A	2609	U
1	1A	2611	U
1	1A	2612	C
1	1A	2629	A
1	1A	2630	G
1	1A	2637	U
1	1A	2654	A
1	1A	2686	G
1	1A	2689	U
1	1A	2690	C
1	1A	2691	C
1	1A	2703	C
1	1A	2712(A)	A

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Mol	Chain	Res	Type
1	1A	2713	A
1	1A	2714	G
1	1A	2721	A
1	1A	2726	U
1	1A	2733	A
1	1A	2757	A
1	1A	2758	A
1	1A	2761	G
1	1A	2765	A
1	1A	2766	G
1	1A	2778	A
1	1A	2780	G
1	1A	2790	A
1	1A	2791	C
1	1A	2793	G
1	1A	2794	C
1	1A	2802	G
1	1A	2805	G
1	1A	2808	U
1	1A	2820	A
1	1A	2821	A
1	1A	2834	G
1	1A	2835	A
1	1A	2872	G
1	1A	2880	C
1	1A	2892	A
1	1A	2894	G
2	1B	2	C
2	1B	25	A
2	1B	35	U
2	1B	45	A
2	1B	56	G
2	1B	67	G
2	1B	73	A
2	1B	110	G
32	1a	7	G
32	1a	9	G
32	1a	32	A
32	1a	39	G
32	1a	47	C
32	1a	48	C
32	1a	51	A

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Mol	Chain	Res	Type
32	1a	54	C
32	1a	61	G
32	1a	78	G
32	1a	91	C
32	1a	96	U
32	1a	98	G
32	1a	101	A
32	1a	116	A
32	1a	121	C
32	1a	131	C
32	1a	146	G
32	1a	159	G
32	1a	163	C
32	1a	174	C
32	1a	180	U
32	1a	182	U
32	1a	195	A
32	1a	197	A
32	1a	202	U
32	1a	203	U
32	1a	204	U
32	1a	216	G
32	1a	217	C
32	1a	243	A
32	1a	247	G
32	1a	251	G
32	1a	258	G
32	1a	266	G
32	1a	267	C
32	1a	289	G
32	1a	321	A
32	1a	328	C
32	1a	332	G
32	1a	344	A
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	384	G
32	1a	397	A

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Mol	Chain	Res	Type
32	1a	398	C
32	1a	406	G
32	1a	412	A
32	1a	424	G
32	1a	429	U
32	1a	441	A
32	1a	442	C
32	1a	452	A
32	1a	461	A
32	1a	470	C
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	527	7MG
32	1a	531	U
32	1a	532	A
32	1a	533	A
32	1a	547	A
32	1a	559	A
32	1a	561	U
32	1a	562	C
32	1a	568	G
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	577	G
32	1a	596	C
32	1a	630	G
32	1a	653	A
32	1a	665	A
32	1a	673	G
32	1a	687	A
32	1a	688	G
32	1a	695	A
32	1a	702	A
32	1a	723	U
32	1a	731	G

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Mol	Chain	Res	Type
32	1a	749	C
32	1a	755	G
32	1a	759	A
32	1a	773	G
32	1a	777	A
32	1a	792	A
32	1a	793	U
32	1a	794	A
32	1a	815	A
32	1a	816	A
32	1a	817	C
32	1a	821	G
32	1a	828	A
32	1a	840	C
32	1a	841	U
32	1a	851	G
32	1a	859	A
32	1a	870	U
32	1a	885	G
32	1a	902	G
32	1a	914	A
32	1a	926	G
32	1a	927	G
32	1a	931	C
32	1a	934	C
32	1a	960	U
32	1a	961	U
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	972	C
32	1a	974	A
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	992	U
32	1a	993	G
32	1a	1001	A
32	1a	1001(A)	G
32	1a	1003	G
32	1a	1005	A
32	1a	1006	C

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Mol	Chain	Res	Type
32	1a	1009	G
32	1a	1020	U
32	1a	1021	G
32	1a	1022	G
32	1a	1023	G
32	1a	1025	U
32	1a	1026	G
32	1a	1027	C
32	1a	1028	C
32	1a	1029	C
32	1a	1030	C
32	1a	1030(A)	G
32	1a	1030(C)	G
32	1a	1031	G
32	1a	1032	G
32	1a	1033	G
32	1a	1039	C
32	1a	1043	C
32	1a	1054	C
32	1a	1065	U
32	1a	1066	C
32	1a	1068	G
32	1a	1081	G
32	1a	1087	G
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1104	G
32	1a	1108	G
32	1a	1123	A
32	1a	1125	U
32	1a	1134	G
32	1a	1135	U
32	1a	1136	U
32	1a	1137	C
32	1a	1138	G
32	1a	1139	G
32	1a	1140	C
32	1a	1141	C
32	1a	1146	A
32	1a	1152	A
32	1a	1157	A

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Mol	Chain	Res	Type
32	1a	1159	U
32	1a	1183	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	1222	G
32	1a	1227	A
32	1a	1236	A
32	1a	1238	A
32	1a	1240	U
32	1a	1241	G
32	1a	1256	A
32	1a	1257	U
32	1a	1258	G
32	1a	1260	C
32	1a	1269	A
32	1a	1270	C
32	1a	1278	U
32	1a	1279	A
32	1a	1280	A
32	1a	1286	A
32	1a	1287	A
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1305	G
32	1a	1320	C
32	1a	1338	G
32	1a	1346	A
32	1a	1347	G
32	1a	1363	C
32	1a	1370	G
32	1a	1419	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1446	U
32	1a	1447	A
32	1a	1452	C
32	1a	1487	G

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Mol	Chain	Res	Type
32	1a	1492	A
32	1a	1494	G
32	1a	1503	A
32	1a	1504	G
32	1a	1506	U
32	1a	1517	G
32	1a	1529	G
32	1a	1530	G
32	1a	1532	U
53	1v	13	A
53	1v	14	A
53	1v	24	A
54	1w	3	C
54	1w	7	A
54	1w	10	G
54	1w	19	G
54	1w	21	A
54	1w	22	G
54	1w	23	A
54	1w	24	G
54	1w	46	7MG
54	1w	47	U
54	1w	48	C
54	1w	59	U
54	1w	62	C
54	1w	68	C
54	1w	72	C
54	1w	73	A
54	1w	75	C
54	1w	76	A
55	1x	6	G
55	1x	9	G
55	1x	19	G
55	1x	20	U
55	1x	21	A
55	1x	34	C
55	1x	42	G
55	1x	48	C
55	1x	67	C
55	1x	76	A
54	1y	2	C
54	1y	5	G

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Mol	Chain	Res	Type
54	1y	9	A
54	1y	11	C
54	1y	13	C
54	1y	19	G
54	1y	20	U
54	1y	21	A
54	1y	22	G
54	1y	26	A
54	1y	33	U
54	1y	34	G
54	1y	39	PSU
54	1y	44	G
54	1y	45	U
54	1y	46	7MG
54	1y	47	U
54	1y	48	C
54	1y	56	C
54	1y	57	G
54	1y	58	A
54	1y	65	G
54	1y	70	G
1	2A	12	U
1	2A	15	G
1	2A	35	G
1	2A	45	C
1	2A	55	G
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	79	G
1	2A	84	A
1	2A	90	U
1	2A	95	G
1	2A	96	G
1	2A	100	G
1	2A	102	G
1	2A	118	A
1	2A	119	A
1	2A	120	U
1	2A	131	G
1	2A	154(A)	C
1	2A	157	U

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Mol	Chain	Res	Type
1	2A	181	A
1	2A	196	A
1	2A	198	C
1	2A	199	A
1	2A	205	G
1	2A	214	G
1	2A	215	G
1	2A	216	A
1	2A	219	G
1	2A	221	A
1	2A	222	A
1	2A	227	A
1	2A	228	A
1	2A	229	A
1	2A	232	G
1	2A	233	A
1	2A	248	G
1	2A	266	G
1	2A	271(A)	A
1	2A	271(E)	U
1	2A	271(F)	C
1	2A	271(I)	G
1	2A	271(K)	U
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	272(B)	G
1	2A	277	C
1	2A	278	A
1	2A	294	A
1	2A	311	A
1	2A	327	G
1	2A	328	U
1	2A	329	G
1	2A	330	A
1	2A	333	G
1	2A	338	G
1	2A	342	G
1	2A	348	G
1	2A	352	G
1	2A	354	G
1	2A	362	U

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Mol	Chain	Res	Type
1	2A	363	G
1	2A	363(B)	G
1	2A	370	G
1	2A	386	G
1	2A	396	G
1	2A	402	A
1	2A	405	U
1	2A	411	G
1	2A	412	A
1	2A	422	A
1	2A	435	C
1	2A	442	G
1	2A	443	A
1	2A	444	C
1	2A	454	A
1	2A	455	C
1	2A	457	A
1	2A	470	A
1	2A	481	G
1	2A	505	A
1	2A	508	G
1	2A	509	C
1	2A	517	C
1	2A	529	A
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	533	G
1	2A	545	G
1	2A	562	U
1	2A	563	G
1	2A	573	G
1	2A	574	C
1	2A	575	A
1	2A	587	C
1	2A	588	U
1	2A	592	G
1	2A	599	G
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	614(B)	G

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Mol	Chain	Res	Type
1	2A	614(C)	A
1	2A	615	G
1	2A	616	G
1	2A	627	A
1	2A	634	C
1	2A	637	A
1	2A	645	C
1	2A	646	A
1	2A	647	G
1	2A	652(B)	A
1	2A	652(C)	G
1	2A	653	A
1	2A	661	C
1	2A	669	G
1	2A	686	G
1	2A	717	G
1	2A	722	A
1	2A	726	G
1	2A	730	C
1	2A	752	A
1	2A	753	C
1	2A	771	G
1	2A	775	G
1	2A	776	G
1	2A	782	A
1	2A	784	A
1	2A	785	G
1	2A	790	C
1	2A	792	G
1	2A	794	G
1	2A	805	G
1	2A	811	U
1	2A	812	C
1	2A	819	A
1	2A	827	U
1	2A	828	U
1	2A	847	U
1	2A	848	G
1	2A	857	C
1	2A	859	G
1	2A	864	G
1	2A	866	A

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Mol	Chain	Res	Type
1	2A	867	C
1	2A	869	G
1	2A	874	G
1	2A	875	G
1	2A	878	A
1	2A	879	G
1	2A	880	G
1	2A	884	C
1	2A	886	C
1	2A	887	A
1	2A	888	C
1	2A	889	C
1	2A	893	C
1	2A	894	C
1	2A	896	A
1	2A	897	C
1	2A	900	A
1	2A	901	A
1	2A	910	A
1	2A	917	A
1	2A	923	C
1	2A	932	G
1	2A	933	A
1	2A	941	A
1	2A	943	U
1	2A	945	A
1	2A	946	G
1	2A	951	C
1	2A	952	G
1	2A	953	A
1	2A	957	A
1	2A	961	C
1	2A	974	G
1	2A	975	C
1	2A	983	A
1	2A	996	A
1	2A	1005	C
1	2A	1012	U
1	2A	1013	C
1	2A	1017	G
1	2A	1022	G
1	2A	1026	U

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Mol	Chain	Res	Type
1	2A	1027	A
1	2A	1033	U
1	2A	1036	G
1	2A	1038	C
1	2A	1039	G
1	2A	1043	C
1	2A	1114	G
1	2A	1116	C
1	2A	1118	C
1	2A	1126	A
1	2A	1130	U
1	2A	1133	U
1	2A	1135	C
1	2A	1136	G
1	2A	1137	G
1	2A	1139	G
1	2A	1144	G
1	2A	1155	A
1	2A	1166	C
1	2A	1171	G
1	2A	1183	G
1	2A	1198	U
1	2A	1205	U
1	2A	1210	A
1	2A	1211	U
1	2A	1212	G
1	2A	1220	A
1	2A	1227	G
1	2A	1229	G
1	2A	1237	A
1	2A	1250	G
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A
1	2A	1273	U
1	2A	1284	A
1	2A	1300	U
1	2A	1301	A
1	2A	1303	G
1	2A	1306	C
1	2A	1314	C

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Mol	Chain	Res	Type
1	2A	1318	C
1	2A	1332	G
1	2A	1342	A
1	2A	1345	C
1	2A	1359	A
1	2A	1360	A
1	2A	1365	A
1	2A	1368	G
1	2A	1370	C
1	2A	1373	A
1	2A	1380	G
1	2A	1384	A
1	2A	1385	G
1	2A	1386	C
1	2A	1416	G
1	2A	1417	C
1	2A	1420	U
1	2A	1421	G
1	2A	1427	A
1	2A	1428	C
1	2A	1429	G
1	2A	1437	C
1	2A	1445	A
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	1479	G
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	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1516	C
1	2A	1525	G

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Mol	Chain	Res	Type
1	2A	1531	C
1	2A	1532	C
1	2A	1533	G
1	2A	1541	G
1	2A	1545	A
1	2A	1547	C
1	2A	1558	A
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1583	A
1	2A	1584	C
1	2A	1592	C
1	2A	1603	A
1	2A	1608	A
1	2A	1609	A
1	2A	1610	A
1	2A	1616	A
1	2A	1640	C
1	2A	1648	C
1	2A	1650	G
1	2A	1654	A
1	2A	1664	A
1	2A	1674	G
1	2A	1675	C
1	2A	1696	G
1	2A	1700	A
1	2A	1701	A
1	2A	1721	G
1	2A	1722	A
1	2A	1741	A
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	1777	U
1	2A	1780	A
1	2A	1786	A
1	2A	1791	A

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Mol	Chain	Res	Type
1	2A	1800	C
1	2A	1801	G
1	2A	1812	A
1	2A	1816	G
1	2A	1829	A
1	2A	1835	G
1	2A	1847	A
1	2A	1848	A
1	2A	1858	G
1	2A	1877	A
1	2A	1878	G
1	2A	1900	A
1	2A	1906	G
1	2A	1913	A
1	2A	1914	C
1	2A	1929	G
1	2A	1930	G
1	2A	1931	U
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	1992	G
1	2A	1993	U
1	2A	1997	G
1	2A	2020	A
1	2A	2023	G
1	2A	2031	A
1	2A	2032	G
1	2A	2033	A
1	2A	2043	C
1	2A	2050	C
1	2A	2055	C
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G
1	2A	2062	A

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Mol	Chain	Res	Type
1	2A	2069	G
1	2A	2093	G
1	2A	2105	C
1	2A	2108	C
1	2A	2110	G
1	2A	2111	C
1	2A	2112	G
1	2A	2116	G
1	2A	2119	A
1	2A	2122	U
1	2A	2124	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	2139	C
1	2A	2141	G
1	2A	2142	C
1	2A	2146	C
1	2A	2150	U
1	2A	2153	G
1	2A	2155	G
1	2A	2157	G
1	2A	2158	A
1	2A	2163	C
1	2A	2165	G
1	2A	2166	G
1	2A	2167	U
1	2A	2168	G
1	2A	2171	A
1	2A	2172	U
1	2A	2173	A
1	2A	2174	C
1	2A	2178	C
1	2A	2181	G
1	2A	2185	C

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Mol	Chain	Res	Type
1	2A	2192	G
1	2A	2198	A
1	2A	2200	C
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2218	U
1	2A	2225	A
1	2A	2239	G
1	2A	2248	C
1	2A	2267	A
1	2A	2268	A
1	2A	2272	U
1	2A	2275	C
1	2A	2279	G
1	2A	2282	G
1	2A	2283	C
1	2A	2287	A
1	2A	2305	A
1	2A	2308	G
1	2A	2310	A
1	2A	2311	A
1	2A	2312	U
1	2A	2319	G
1	2A	2320	A
1	2A	2325	G
1	2A	2327	A
1	2A	2334	G
1	2A	2336	A
1	2A	2347	C
1	2A	2350	C
1	2A	2354	G
1	2A	2376	A
1	2A	2377	A
1	2A	2383	G
1	2A	2385	C
1	2A	2388	A
1	2A	2400	G
1	2A	2402	C
1	2A	2403	C
1	2A	2406	U
1	2A	2425	A

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Mol	Chain	Res	Type
1	2A	2429	G
1	2A	2430	A
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2448	A
1	2A	2465	C
1	2A	2469	A
1	2A	2474	C
1	2A	2476	A
1	2A	2484	G
1	2A	2487	G
1	2A	2489	G
1	2A	2490	G
1	2A	2491	U
1	2A	2494	G
1	2A	2502	G
1	2A	2504	U
1	2A	2505	G
1	2A	2506	U
1	2A	2518	A
1	2A	2520	C
1	2A	2525	G
1	2A	2528	U
1	2A	2532	G
1	2A	2554	U
1	2A	2566	A
1	2A	2567	G
1	2A	2573	C
1	2A	2602	A
1	2A	2611	U
1	2A	2612	C
1	2A	2615	U
1	2A	2629	A
1	2A	2630	G
1	2A	2661	G
1	2A	2663	G
1	2A	2669	G
1	2A	2673	G
1	2A	2674	G
1	2A	2689	U
1	2A	2690	C

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Mol	Chain	Res	Type
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G
1	2A	2726	U
1	2A	2733	A
1	2A	2744	G
1	2A	2745	C
1	2A	2751	G
1	2A	2757	A
1	2A	2759	G
1	2A	2761	G
1	2A	2764	A
1	2A	2765	A
1	2A	2778	A
1	2A	2779	U
1	2A	2793	G
1	2A	2794	C
1	2A	2804	C
1	2A	2808	U
1	2A	2818	G
1	2A	2820	A
1	2A	2821	A
1	2A	2833	G
1	2A	2835	A
1	2A	2849	U
1	2A	2872	G
1	2A	2875	C
1	2A	2879	C
1	2A	2880	C
1	2A	2893	G
1	2A	2894	G
1	2A	2895	U
1	2A	2897	U
2	2B	2	C
2	2B	7	G
2	2B	8	U
2	2B	9	G
2	2B	13	A
2	2B	17	C
2	2B	20	C
2	2B	24	G
2	2B	25	A

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Mol	Chain	Res	Type
2	2B	30	C
2	2B	32	C
2	2B	34	U
2	2B	35	U
2	2B	42	C
2	2B	45	A
2	2B	46	A
2	2B	52	A
2	2B	53	A
2	2B	56	G
2	2B	57	A
2	2B	65	C
2	2B	66	A
2	2B	67	G
2	2B	73	A
2	2B	74	U
2	2B	75	G
2	2B	83	G
2	2B	85	G
2	2B	88	C
2	2B	91	C
2	2B	94	C
2	2B	101	G
2	2B	106	G
2	2B	108	U
2	2B	110	G
2	2B	116	G
32	2a	7	G
32	2a	9	G
32	2a	32	A
32	2a	39	G
32	2a	47	C
32	2a	48	C
32	2a	51	A
32	2a	52	G
32	2a	66	G
32	2a	78	G
32	2a	80	G
32	2a	88	A
32	2a	89	C
32	2a	90	U
32	2a	96	U

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Mol	Chain	Res	Type
32	2a	98	G
32	2a	101	A
32	2a	116	A
32	2a	121	C
32	2a	131	C
32	2a	146	G
32	2a	159	G
32	2a	163	C
32	2a	174	C
32	2a	180	U
32	2a	182	U
32	2a	195	A
32	2a	197	A
32	2a	201	C
32	2a	203	U
32	2a	204	U
32	2a	216	G
32	2a	217	C
32	2a	243	A
32	2a	247	G
32	2a	251	G
32	2a	258	G
32	2a	266	G
32	2a	267	C
32	2a	289	G
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	344	A
32	2a	352	C
32	2a	353	A
32	2a	354	G
32	2a	367	U
32	2a	372	C
32	2a	373	A
32	2a	384	G
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	412	A
32	2a	424	G
32	2a	429	U

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Mol	Chain	Res	Type
32	2a	441	A
32	2a	442	C
32	2a	452	A
32	2a	461	A
32	2a	470	C
32	2a	474	G
32	2a	485	G
32	2a	496	A
32	2a	498	U
32	2a	505	G
32	2a	509	A
32	2a	510	A
32	2a	511	C
32	2a	518	C
32	2a	531	U
32	2a	532	A
32	2a	533	A
32	2a	547	A
32	2a	559	A
32	2a	560	U
32	2a	561	U
32	2a	562	C
32	2a	568	G
32	2a	572	A
32	2a	573	A
32	2a	576	G
32	2a	577	G
32	2a	596	C
32	2a	630	G
32	2a	653	A
32	2a	665	A
32	2a	673	G
32	2a	687	A
32	2a	688	G
32	2a	695	A
32	2a	702	A
32	2a	723	U
32	2a	731	G
32	2a	749	C
32	2a	755	G
32	2a	759	A
32	2a	773	G

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Mol	Chain	Res	Type
32	2a	777	A
32	2a	792	A
32	2a	793	U
32	2a	794	A
32	2a	815	A
32	2a	816	A
32	2a	817	C
32	2a	821	G
32	2a	828	A
32	2a	840	C
32	2a	841	U
32	2a	851	G
32	2a	859	A
32	2a	870	U
32	2a	885	G
32	2a	902	G
32	2a	914	A
32	2a	916	G
32	2a	926	G
32	2a	927	G
32	2a	931	C
32	2a	934	C
32	2a	960	U
32	2a	961	U
32	2a	968	A
32	2a	969	A
32	2a	971	G
32	2a	972	C
32	2a	974	A
32	2a	975	A
32	2a	976	G
32	2a	977	A
32	2a	992	U
32	2a	993	G
32	2a	1000	U
32	2a	1001	A
32	2a	1001(A)	G
32	2a	1002	G
32	2a	1004	A
32	2a	1005	A
32	2a	1006	C
32	2a	1009	G

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Mol	Chain	Res	Type
32	2a	1020	U
32	2a	1021	G
32	2a	1022	G
32	2a	1023	G
32	2a	1025	U
32	2a	1026	G
32	2a	1027	C
32	2a	1030	C
32	2a	1030(A)	G
32	2a	1030(B)	C
32	2a	1030(C)	G
32	2a	1031	G
32	2a	1032	G
32	2a	1033	G
32	2a	1039	C
32	2a	1043	C
32	2a	1054	C
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1077	G
32	2a	1081	G
32	2a	1087	G
32	2a	1094	G
32	2a	1095	U
32	2a	1101	A
32	2a	1104	G
32	2a	1108	G
32	2a	1117	G
32	2a	1125	U
32	2a	1129	C
32	2a	1130	A
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

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Mol	Chain	Res	Type
32	2a	1157	A
32	2a	1159	U
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	1211	U
32	2a	1212	U
32	2a	1213	A
32	2a	1222	G
32	2a	1227	A
32	2a	1236	A
32	2a	1238	A
32	2a	1240	U
32	2a	1241	G
32	2a	1256	A
32	2a	1257	U
32	2a	1258	G
32	2a	1260	C
32	2a	1269	A
32	2a	1270	C
32	2a	1278	U
32	2a	1279	A
32	2a	1280	A
32	2a	1287	A
32	2a	1300	G
32	2a	1305	G
32	2a	1320	C
32	2a	1338	G
32	2a	1346	A
32	2a	1347	G
32	2a	1363	C
32	2a	1368	G
32	2a	1370	G
32	2a	1400	5MC
32	2a	1401	G
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1446	U

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Mol	Chain	Res	Type
32	2a	1447	A
32	2a	1452	C
32	2a	1456	G
32	2a	1487	G
32	2a	1492	A
32	2a	1494	G
32	2a	1503	A
32	2a	1504	G
32	2a	1506	U
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	24	A
54	2w	3	C
54	2w	4	C
54	2w	7	A
54	2w	8	4SU
54	2w	9	A
54	2w	10	G
54	2w	19	G
54	2w	21	A
54	2w	22	G
54	2w	24	G
54	2w	46	7MG
54	2w	48	C
54	2w	59	U
54	2w	62	C
54	2w	68	C
54	2w	71	G
54	2w	72	C
54	2w	73	A
54	2w	75	C
54	2w	76	A
55	2x	19	G
55	2x	21	A
55	2x	42	G
55	2x	47	U

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Mol	Chain	Res	Type
55	2x	48	C
55	2x	56	C
55	2x	67	C
55	2x	68	C
55	2x	76	A
54	2y	2	C
54	2y	9	A
54	2y	13	C
54	2y	19	G
54	2y	22	G
54	2y	33	U
54	2y	34	G
54	2y	39	PSU
54	2y	44	G
54	2y	46	7MG
54	2y	47	U
54	2y	52	G
54	2y	56	C
54	2y	57	G
54	2y	58	A
54	2y	65	G
54	2y	70	G

All (64) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	90	U
1	1A	196	A
1	1A	266	G
1	1A	271(K)	U
1	1A	278	A
1	1A	548	A
1	1A	746	A
1	1A	764	A
1	1A	839	U
1	1A	896	A
1	1A	974	G
1	1A	1047	G
1	1A	1065	U
1	1A	1067	A
1	1A	1089	G
1	1A	1174	A

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Mol	Chain	Res	Type
1	1A	1175	U
1	1A	1176	G
1	1A	1210	A
1	1A	1275	A
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	2131	G
1	1A	2181	G
1	1A	2183	C
1	1A	2430	A
1	1A	2629	A
1	1A	2689	U
1	1A	2756	U
2	1B	1	U
1	2A	196	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	528	A
1	2A	530	G
1	2A	587	C
1	2A	752	A
1	2A	839	U
1	2A	856	C
1	2A	893	C
1	2A	900	A
1	2A	1026	U
1	2A	1210	A
1	2A	1300	U
1	2A	1379	A
1	2A	1420	U
1	2A	1442	G
1	2A	1493	C
1	2A	1530	C
1	2A	1653	G
1	2A	1913	A

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Mol	Chain	Res	Type
1	2A	1992	G
1	2A	2126	A
1	2A	2156	G
1	2A	2406	U
1	2A	2689	U
1	2A	2756	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	PSU	1A	2605	1	17,21,22	1.62	3 (17%)	20,30,33	3.15	6 (30%)
54	4SU	2w	8	54,56	14,21,22	1.24	1 (7%)	15,30,33	1.63	2 (13%)
32	2MG	2a	1207	32	19,26,27	1.22	2 (10%)	21,38,41	2.27	8 (38%)
32	5MC	1a	1407	32	15,22,23	1.28	1 (6%)	19,32,35	1.30	2 (10%)
1	5MU	1A	1939	1,56	15,22,23	1.00	1 (6%)	16,32,35	1.87	2 (12%)
1	5MC	1A	1962	1	15,22,23	1.35	1 (6%)	19,32,35	1.27	3 (15%)
54	PSU	1y	32	54	17,21,22	1.47	2 (11%)	20,30,33	3.16	5 (25%)
54	4SU	1y	8	54	14,21,22	1.38	2 (14%)	15,30,33	1.47	2 (13%)
54	4SU	1w	8	54	14,21,22	1.22	1 (7%)	15,30,33	1.54	2 (13%)
54	5MU	1w	54	54	15,22,23	1.05	2 (13%)	16,32,35	1.98	2 (12%)
1	4OC	1A	1920	1	15,22,24	0.69	0	17,31,35	1.63	3 (17%)
32	7MG	2a	527	32,56	22,26,27	1.77	4 (18%)	28,39,42	2.68	9 (32%)
43	0TD	2l	92	43	4,9,10	3.21	1 (25%)	3,11,13	6.53	1 (33%)
1	5MU	2A	1915	1	15,22,23	1.09	1 (6%)	16,32,35	1.85	2 (12%)
1	OMG	1A	2251	55,1,56	18,26,27	1.25	2 (11%)	20,38,41	2.38	6 (30%)
54	PSU	1y	55	54	17,21,22	1.46	3 (17%)	20,30,33	3.13	5 (25%)
32	MA6	2a	1518	32	19,26,27	0.97	1 (5%)	18,38,41	1.70	4 (22%)
32	5MC	1a	967	32	15,22,23	1.34	1 (6%)	19,32,35	1.30	3 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MC	2A	1942	1	15,22,23	1.30	1 (6%)	19,32,35	1.42	3 (15%)
1	5MU	1A	1915	1	15,22,23	1.08	1 (6%)	16,32,35	1.76	2 (12%)
32	M2G	2a	966	32	20,27,28	1.44	3 (15%)	22,40,43	2.18	5 (22%)
54	PSU	2y	55	54	17,21,22	1.55	3 (17%)	20,30,33	3.14	6 (30%)
32	UR3	2a	1498	32	14,22,23	0.79	1 (7%)	15,32,35	0.78	1 (6%)
1	PSU	1A	1911	1	17,21,22	1.59	3 (17%)	20,30,33	3.17	6 (30%)
54	PSU	2w	39	54	17,21,22	1.48	3 (17%)	20,30,33	3.43	5 (25%)
55	4SU	1x	8	55	14,21,22	1.42	2 (14%)	15,30,33	2.40	2 (13%)
55	PSU	2x	55	55	17,21,22	1.58	3 (17%)	20,30,33	3.15	5 (25%)
32	5MC	1a	1400	32	15,22,23	1.44	1 (6%)	19,32,35	1.26	3 (15%)
54	MIA	2y	37	54	18,24,32	1.17	2 (11%)	18,35,47	1.27	2 (11%)
54	PSU	2y	32	54	17,21,22	1.42	2 (11%)	20,30,33	3.22	5 (25%)
32	5MC	2a	1400	32	15,22,23	1.27	1 (6%)	19,32,35	1.37	2 (10%)
1	PSU	2A	1911	1	17,21,22	1.56	3 (17%)	20,30,33	3.15	6 (30%)
55	5MU	1x	54	55,56	15,22,23	1.08	1 (6%)	16,32,35	2.09	2 (12%)
54	7MG	2w	46	54	22,26,27	1.78	4 (18%)	28,39,42	2.56	9 (32%)
1	2MU	1A	2552	1,56	14,22,24	0.93	1 (7%)	14,31,36	0.74	1 (7%)
55	PSU	1x	55	55	17,21,22	1.76	3 (17%)	20,30,33	3.23	6 (30%)
32	M2G	1a	966	32	20,27,28	1.35	3 (15%)	22,40,43	2.13	6 (27%)
32	2MG	1a	1207	32	19,26,27	1.26	2 (10%)	21,38,41	2.41	9 (42%)
54	7MG	2y	46	54	22,26,27	1.78	4 (18%)	28,39,42	2.76	13 (46%)
1	5MU	2A	1939	1,56	15,22,23	1.10	2 (13%)	16,32,35	1.74	2 (12%)
54	PSU	2y	39	54	17,21,22	1.62	4 (23%)	20,30,33	2.84	8 (40%)
54	5MU	2y	54	54	15,22,23	1.08	1 (6%)	16,32,35	2.12	1 (6%)
1	PSU	2A	1917	1	17,21,22	1.55	2 (11%)	20,30,33	3.28	6 (30%)
43	0TD	1l	92	43	4,9,10	3.28	1 (25%)	3,11,13	10.66	1 (33%)
54	7MG	1w	46	54	22,26,27	1.72	4 (18%)	28,39,42	2.79	9 (32%)
1	OMG	2A	2251	55,1,56	18,26,27	1.21	2 (11%)	20,38,41	2.07	6 (30%)
54	PSU	1w	39	54	17,21,22	1.53	2 (11%)	20,30,33	3.18	6 (30%)
32	5MC	1a	1404	32	15,22,23	1.33	1 (6%)	19,32,35	1.36	3 (15%)
1	4OC	2A	1920	1	15,22,24	0.63	0	17,31,35	1.38	2 (11%)
32	MA6	2a	1519	32	19,26,27	0.99	1 (5%)	18,38,41	1.61	3 (16%)
55	5MU	2x	54	55	15,22,23	1.10	1 (6%)	16,32,35	1.80	2 (12%)
32	MA6	1a	1519	32	19,26,27	1.03	1 (5%)	18,38,41	1.65	4 (22%)
54	PSU	1y	39	54	17,21,22	1.56	3 (17%)	20,30,33	3.25	6 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
54	PSU	2w	55	54	17,21,22	1.39	2 (11%)	20,30,33	3.30	6 (30%)
54	MIA	2w	37	54	18,24,32	1.10	2 (11%)	18,35,47	1.25	2 (11%)
1	2MU	2A	2552	1,56	14,22,24	0.93	0	14,31,36	0.87	1 (7%)
54	MIA	1w	37	54	24,31,32	2.22	3 (12%)	26,44,47	2.46	8 (30%)
54	5MU	2w	54	54	15,22,23	1.08	1 (6%)	16,32,35	2.21	1 (6%)
54	7MG	1y	46	54	22,26,27	1.81	3 (13%)	28,39,42	2.78	9 (32%)
32	5MC	2a	967	32,56	15,22,23	1.32	1 (6%)	19,32,35	1.37	3 (15%)
1	5MC	1A	1942	1	15,22,23	1.18	1 (6%)	19,32,35	1.51	3 (15%)
32	4OC	1a	1402	32	16,23,24	0.66	0	17,32,35	1.26	1 (5%)
32	5MC	2a	1407	32	15,22,23	1.30	1 (6%)	19,32,35	1.41	2 (10%)
32	4OC	2a	1402	32	16,23,24	0.61	0	17,32,35	1.51	1 (5%)
55	4SU	2x	8	55	14,21,22	1.24	2 (14%)	15,30,33	2.44	2 (13%)
55	5MC	2x	32	55	15,22,23	1.28	1 (6%)	19,32,35	1.33	2 (10%)
55	5MC	1x	32	55	15,22,23	1.34	1 (6%)	19,32,35	1.34	3 (15%)
54	PSU	1w	55	54	17,21,22	1.45	2 (11%)	20,30,33	3.27	6 (30%)
54	5MU	1y	54	54	15,22,23	0.99	1 (6%)	16,32,35	2.49	1 (6%)
54	4SU	2y	8	54	14,21,22	1.31	1 (7%)	15,30,33	1.50	2 (13%)
54	PSU	2w	32	54	17,21,22	1.57	2 (11%)	20,30,33	3.22	6 (30%)
1	PSU	2A	2605	1	17,21,22	1.53	2 (11%)	20,30,33	2.83	6 (30%)
32	PSU	1a	516	32,56	17,21,22	1.52	3 (17%)	20,30,33	3.02	6 (30%)
1	2MA	1A	2503	1,56	17,25,26	1.29	2 (11%)	19,37,40	2.07	3 (15%)
32	PSU	2a	516	32	17,21,22	1.48	3 (17%)	20,30,33	3.08	6 (30%)
32	MA6	1a	1518	32	19,26,27	1.02	2 (10%)	18,38,41	1.69	5 (27%)
54	PSU	1w	32	54	17,21,22	1.45	2 (11%)	20,30,33	3.11	5 (25%)
1	2MA	2A	2503	1,56	17,25,26	1.25	2 (11%)	19,37,40	1.94	4 (21%)
1	PSU	1A	1917	1	17,21,22	1.54	3 (17%)	20,30,33	3.10	6 (30%)
32	7MG	1a	527	32,56	22,26,27	1.79	4 (18%)	28,39,42	2.76	10 (35%)
1	5MC	2A	1962	1,56	15,22,23	1.27	1 (6%)	19,32,35	1.36	3 (15%)
32	UR3	1a	1498	32	14,22,23	0.84	1 (7%)	15,32,35	0.86	1 (6%)
54	MIA	1y	37	54	18,24,32	1.13	2 (11%)	18,35,47	1.25	2 (11%)
32	5MC	2a	1404	32	15,22,23	1.36	1 (6%)	19,32,35	1.28	3 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	1A	2605	1	-	0/7/25/26	0/2/2/2
54	4SU	2w	8	54,56	-	0/5/25/26	0/2/2/2
32	2MG	2a	1207	32	-	0/5/27/28	0/3/3/3
32	5MC	1a	1407	32	-	0/5/25/26	0/2/2/2
1	5MU	1A	1939	1,56	-	0/5/25/26	0/2/2/2
1	5MC	1A	1962	1	-	2/5/25/26	0/2/2/2
54	PSU	1y	32	54	-	0/7/25/26	0/2/2/2
54	4SU	1y	8	54	-	0/5/25/26	0/2/2/2
54	4SU	1w	8	54	-	0/5/25/26	0/2/2/2
54	5MU	1w	54	54	-	0/5/25/26	0/2/2/2
1	4OC	1A	1920	1	-	1/7/27/30	0/2/2/2
32	7MG	2a	527	32,56	-	1/7/37/38	0/3/3/3
43	0TD	2l	92	43	-	3/3/12/14	-
1	5MU	2A	1915	1	-	0/5/25/26	0/2/2/2
1	OMG	1A	2251	55,1,56	-	0/5/27/28	0/3/3/3
54	PSU	1y	55	54	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	3/7/29/30	0/3/3/3
32	5MC	1a	967	32	-	0/5/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/5/25/26	0/2/2/2
1	5MU	1A	1915	1	-	2/5/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
54	PSU	2y	55	54	-	2/7/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/5/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/5/25/26	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	2/5/25/26	0/2/2/2
54	MIA	2y	37	54	-	2/3/25/34	0/3/3/3
54	PSU	2y	32	54	-	0/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	1/5/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
55	5MU	1x	54	55,56	-	0/5/25/26	0/2/2/2
54	7MG	2w	46	54	-	2/7/37/38	0/3/3/3
1	2MU	1A	2552	1,56	-	0/7/27/28	0/2/2/2
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
32	2MG	1a	1207	32	-	2/5/27/28	0/3/3/3
54	7MG	2y	46	54	-	5/7/37/38	0/3/3/3
1	5MU	2A	1939	1,56	-	2/5/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	PSU	2y	39	54	-	2/7/25/26	0/2/2/2
54	5MU	2y	54	54	-	0/5/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	2/3/12/14	-
54	7MG	1w	46	54	-	1/7/37/38	0/3/3/3
1	OMG	2A	2251	55,1,56	-	1/5/27/28	0/3/3/3
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/5/25/26	0/2/2/2
1	4OC	2A	1920	1	-	0/7/27/30	0/2/2/2
32	MA6	2a	1519	32	-	6/7/29/30	0/3/3/3
55	5MU	2x	54	55	-	0/5/25/26	0/2/2/2
32	MA6	1a	1519	32	-	4/7/29/30	0/3/3/3
54	PSU	1y	39	54	-	2/7/25/26	0/2/2/2
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
54	MIA	2w	37	54	-	0/3/25/34	0/3/3/3
1	2MU	2A	2552	1,56	-	0/7/27/28	0/2/2/2
54	MIA	1w	37	54	-	3/11/33/34	0/3/3/3
54	5MU	2w	54	54	-	0/5/25/26	0/2/2/2
54	7MG	1y	46	54	-	6/7/37/38	0/3/3/3
32	5MC	2a	967	32,56	-	2/5/25/26	0/2/2/2
1	5MC	1A	1942	1	-	0/5/25/26	0/2/2/2
32	4OC	1a	1402	32	-	3/9/29/30	0/2/2/2
32	5MC	2a	1407	32	-	0/5/25/26	0/2/2/2
32	4OC	2a	1402	32	-	3/9/29/30	0/2/2/2
55	4SU	2x	8	55	-	1/5/25/26	0/2/2/2
55	5MC	2x	32	55	-	2/5/25/26	0/2/2/2
55	5MC	1x	32	55	-	0/5/25/26	0/2/2/2
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
54	5MU	1y	54	54	-	0/5/25/26	0/2/2/2
54	4SU	2y	8	54	-	1/5/25/26	0/2/2/2
54	PSU	2w	32	54	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	32,56	-	0/7/25/26	0/2/2/2
1	2MA	1A	2503	1,56	-	2/3/25/26	0/3/3/3
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	1/7/29/30	0/3/3/3
54	PSU	1w	32	54	-	1/7/25/26	0/2/2/2
1	2MA	2A	2503	1,56	-	1/3/25/26	0/3/3/3
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	7MG	1a	527	32,56	-	3/7/37/38	0/3/3/3
1	5MC	2A	1962	1,56	-	2/5/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/5/25/26	0/2/2/2
54	MIA	1y	37	54	-	0/3/25/34	0/3/3/3
32	5MC	2a	1404	32	-	0/5/25/26	0/2/2/2

All (153) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	37	MIA	C13-C14	7.18	1.53	1.32
54	1w	37	MIA	C2-S10	-6.73	1.70	1.75
43	2l	92	0TD	CB-SB	-6.19	1.69	1.84
43	1l	92	0TD	CB-SB	-6.16	1.69	1.84
55	1x	55	PSU	C5-C1'	-5.30	1.47	1.52
54	2w	46	7MG	C5-C6	5.18	1.48	1.41
54	1y	46	7MG	C5-C6	5.17	1.48	1.41
54	2y	46	7MG	C5-C6	5.15	1.48	1.41
32	1a	1400	5MC	C5-C4	5.13	1.49	1.41
32	2a	1404	5MC	C5-C4	4.89	1.48	1.41
32	2a	527	7MG	C5-C6	4.87	1.48	1.41
1	1A	1962	5MC	C5-C4	4.86	1.48	1.41
55	1x	32	5MC	C5-C4	4.81	1.48	1.41
32	1a	967	5MC	C5-C4	4.80	1.48	1.41
32	2a	967	5MC	C5-C4	4.75	1.48	1.41
32	1a	527	7MG	C5-C6	4.73	1.47	1.41
32	1a	1404	5MC	C5-C4	4.71	1.48	1.41
54	1y	46	7MG	C5-C4	4.67	1.48	1.39
1	2A	1942	5MC	C5-C4	4.64	1.48	1.41
32	1a	527	7MG	C5-C4	4.59	1.48	1.39
32	2a	1407	5MC	C5-C4	4.56	1.48	1.41
1	1A	2605	PSU	C5-C1'	-4.55	1.48	1.52
55	2x	32	5MC	C5-C4	4.51	1.48	1.41
32	2a	527	7MG	C5-C4	4.46	1.47	1.39
32	1a	1407	5MC	C5-C4	4.43	1.48	1.41
32	2a	1400	5MC	C5-C4	4.42	1.48	1.41
1	2A	1962	5MC	C5-C4	4.41	1.48	1.41
32	2a	966	M2G	C5-C6	4.37	1.48	1.41
54	2y	46	7MG	C5-C4	4.35	1.47	1.39
1	2A	1911	PSU	C5-C1'	-4.32	1.48	1.52
54	1w	46	7MG	C5-C4	4.30	1.47	1.39
32	2a	1207	2MG	C5-C6	4.28	1.48	1.41
1	2A	2605	PSU	C5-C1'	-4.28	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1y	8	4SU	C4-S4	-4.27	1.59	1.67
55	2x	55	PSU	C5-C1'	-4.26	1.48	1.52
1	1A	2503	2MA	C5-C6	4.25	1.47	1.41
54	1w	46	7MG	C5-C6	4.25	1.47	1.41
32	1a	1207	2MG	C5-C6	4.24	1.48	1.41
1	1A	1911	PSU	C5-C1'	-4.20	1.48	1.52
54	2w	46	7MG	C5-C4	4.20	1.47	1.39
32	1a	966	M2G	C5-C6	4.19	1.48	1.41
1	2A	2503	2MA	C5-C6	4.12	1.47	1.41
1	1A	1942	5MC	C5-C4	4.12	1.47	1.41
1	1A	1917	PSU	C5-C1'	-4.09	1.48	1.52
54	2y	55	PSU	C5-C1'	-4.08	1.48	1.52
1	1A	2251	OMG	C5-C6	4.08	1.48	1.41
54	2y	8	4SU	C4-S4	-4.06	1.60	1.67
54	2w	32	PSU	C5-C1'	-4.04	1.48	1.52
54	1w	39	PSU	C5-C1'	-4.02	1.48	1.52
1	2A	1917	PSU	C5-C1'	-3.95	1.48	1.52
54	1y	32	PSU	C5-C4	3.91	1.49	1.41
1	2A	2251	OMG	C5-C6	3.89	1.48	1.41
54	2y	39	PSU	C5-C1'	-3.85	1.49	1.52
54	1w	8	4SU	C4-S4	-3.79	1.60	1.67
32	2a	516	PSU	C5-C1'	-3.73	1.49	1.52
32	1a	527	7MG	C5-N7	-3.72	1.33	1.39
54	2w	39	PSU	C5-C1'	-3.71	1.49	1.52
54	2w	32	PSU	C5-C4	3.69	1.49	1.41
54	2w	8	4SU	C4-S4	-3.68	1.60	1.67
55	1x	8	4SU	C4-S4	-3.66	1.60	1.67
32	1a	516	PSU	C5-C1'	-3.66	1.49	1.52
1	2A	1917	PSU	C5-C4	3.65	1.49	1.41
54	2y	39	PSU	C5-C4	3.65	1.49	1.41
54	1y	39	PSU	C5-C1'	-3.63	1.49	1.52
54	1w	32	PSU	C5-C4	3.58	1.49	1.41
54	1y	55	PSU	C5-C1'	-3.57	1.49	1.52
55	2x	55	PSU	C5-C4	3.57	1.49	1.41
55	2x	8	4SU	C4-S4	-3.54	1.61	1.67
54	2y	32	PSU	C5-C4	3.49	1.48	1.41
55	1x	8	4SU	C2-N3	-3.47	1.31	1.38
32	1a	516	PSU	C5-C4	3.46	1.48	1.41
54	1w	55	PSU	C5-C4	3.45	1.48	1.41
54	2y	55	PSU	C5-C4	3.45	1.48	1.41
1	2A	1915	5MU	C5-C4	3.44	1.48	1.41
54	1y	39	PSU	C5-C4	3.43	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1915	5MU	C5-C4	3.42	1.48	1.41
54	2w	55	PSU	C5-C4	3.42	1.48	1.41
55	2x	54	5MU	C5-C4	3.41	1.48	1.41
1	1A	1911	PSU	C5-C4	3.41	1.48	1.41
32	2a	516	PSU	C5-C4	3.39	1.48	1.41
54	1w	32	PSU	C5-C1'	-3.39	1.49	1.52
32	2a	966	M2G	C2-N2	3.38	1.40	1.34
54	1w	46	7MG	C5-N7	-3.38	1.34	1.39
54	1w	55	PSU	C5-C1'	-3.38	1.49	1.52
54	2y	54	5MU	C5-C4	3.37	1.48	1.41
55	1x	54	5MU	C5-C4	3.33	1.48	1.41
54	1y	55	PSU	C5-C4	3.29	1.48	1.41
54	2w	54	5MU	C5-C4	3.29	1.48	1.41
54	2w	39	PSU	C5-C4	3.26	1.48	1.41
1	2A	1939	5MU	C5-C4	3.24	1.48	1.41
54	1y	54	5MU	C5-C4	3.24	1.48	1.41
54	2y	32	PSU	C5-C1'	-3.23	1.49	1.52
1	2A	1911	PSU	C5-C4	3.22	1.48	1.41
54	1y	46	7MG	C5-N7	-3.21	1.34	1.39
55	1x	55	PSU	C5-C4	3.20	1.48	1.41
54	1w	39	PSU	C5-C4	3.20	1.48	1.41
54	2w	55	PSU	C5-C1'	-3.17	1.49	1.52
32	2a	527	7MG	C5-N7	-3.17	1.34	1.39
54	1w	54	5MU	C5-C4	3.16	1.48	1.41
1	2A	2605	PSU	C5-C4	3.15	1.48	1.41
54	2w	46	7MG	C5-N7	-3.12	1.34	1.39
54	1y	32	PSU	C5-C1'	-3.10	1.49	1.52
54	1w	46	7MG	C4-N9	-3.07	1.32	1.38
1	1A	1939	5MU	C5-C4	3.04	1.48	1.41
32	1a	966	M2G	C2-N2	3.00	1.39	1.34
1	1A	1917	PSU	C5-C4	2.99	1.47	1.41
1	1A	2605	PSU	C5-C4	2.98	1.47	1.41
54	2y	46	7MG	C5-N7	-2.86	1.34	1.39
54	2y	37	MIA	C5-C4	2.82	1.48	1.40
54	2y	37	MIA	C2-N3	2.76	1.36	1.32
54	1y	37	MIA	C2-N3	2.74	1.36	1.32
54	2w	46	7MG	C4-N9	-2.69	1.33	1.38
54	1y	37	MIA	C5-C4	2.68	1.48	1.40
54	2w	37	MIA	C5-C4	2.67	1.48	1.40
32	2a	1519	MA6	C5-C4	2.62	1.47	1.40
54	2w	37	MIA	C2-N3	2.60	1.36	1.32
55	2x	8	4SU	C2-N3	-2.57	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1y	39	PSU	O4'-C1'	-2.54	1.40	1.44
32	2a	1518	MA6	C5-C4	2.53	1.47	1.40
32	2a	966	M2G	C5-C4	2.52	1.47	1.40
1	2A	2251	OMG	C5-C4	2.50	1.47	1.40
32	1a	966	M2G	C5-C4	2.47	1.47	1.40
54	1w	37	MIA	C5-C4	2.46	1.47	1.40
1	1A	2251	OMG	C5-C4	2.46	1.47	1.40
32	1a	1498	UR3	C4-N3	2.43	1.41	1.38
32	2a	1207	2MG	C5-C4	2.41	1.47	1.40
32	1a	1518	MA6	C5-C4	2.40	1.47	1.40
54	2y	46	7MG	C4-N9	-2.39	1.33	1.38
1	1A	2605	PSU	C2-N3	-2.37	1.33	1.38
32	1a	1519	MA6	C5-C4	2.37	1.47	1.40
32	1a	1207	2MG	C5-C4	2.34	1.47	1.40
32	1a	527	7MG	C4-N9	-2.30	1.34	1.38
32	1a	516	PSU	O4'-C1'	-2.20	1.41	1.44
1	1A	2503	2MA	C5-C4	2.19	1.46	1.40
55	1x	55	PSU	O4'-C1'	-2.16	1.41	1.44
54	1y	55	PSU	O4'-C1'	-2.15	1.41	1.44
1	2A	2503	2MA	C5-C4	2.15	1.46	1.40
32	2a	527	7MG	C4-N9	-2.15	1.34	1.38
1	1A	2552	2MU	C2-N3	-2.15	1.33	1.38
1	1A	1917	PSU	C2-N3	-2.14	1.33	1.38
54	1y	8	4SU	C2-N3	-2.11	1.34	1.38
1	2A	1911	PSU	O4'-C1'	-2.11	1.41	1.44
54	2w	39	PSU	O4'-C1'	-2.10	1.41	1.44
32	2a	516	PSU	O4'-C1'	-2.08	1.41	1.44
54	2y	55	PSU	O4'-C1'	-2.08	1.41	1.44
1	2A	1939	5MU	C2-N3	-2.08	1.34	1.38
55	2x	55	PSU	O4'-C1'	-2.06	1.41	1.44
1	1A	1911	PSU	C2-N3	-2.06	1.34	1.38
32	2a	1498	UR3	C4-N3	2.05	1.41	1.38
32	1a	1518	MA6	C6-N1	2.04	1.36	1.33
54	2y	39	PSU	O4'-C1'	-2.03	1.41	1.44
54	1w	54	5MU	C2-N3	-2.03	1.34	1.38
54	2y	39	PSU	C2-N1	-2.02	1.34	1.38

All (344) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1l	92	0TD	CSB-SB-CB	18.41	138.07	101.85
43	2l	92	0TD	CSB-SB-CB	-11.25	79.73	101.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2w	39	PSU	N3-C2-N1	-9.73	120.70	128.43
54	1y	54	5MU	C2-N3-C4	9.67	123.31	115.14
32	1a	527	7MG	N3-C4-N9	9.28	138.82	126.91
54	1y	46	7MG	N3-C4-N9	9.23	138.76	126.91
54	2y	32	PSU	N3-C2-N1	-9.06	121.23	128.43
54	1y	55	PSU	N3-C2-N1	-8.80	121.43	128.43
32	2a	527	7MG	N3-C4-N9	8.80	138.21	126.91
1	2A	1917	PSU	N3-C2-N1	-8.79	121.44	128.43
54	1y	32	PSU	N3-C2-N1	-8.78	121.45	128.43
54	2w	55	PSU	N3-C2-N1	-8.74	121.48	128.43
54	1w	46	7MG	N3-C4-N9	8.64	138.00	126.91
55	2x	55	PSU	N3-C2-N1	-8.62	121.58	128.43
54	2y	55	PSU	N3-C2-N1	-8.62	121.58	128.43
54	1w	39	PSU	N3-C2-N1	-8.60	121.60	128.43
32	2a	516	PSU	N3-C2-N1	-8.60	121.60	128.43
1	2A	1911	PSU	N3-C2-N1	-8.58	121.61	128.43
54	2w	32	PSU	N3-C2-N1	-8.57	121.62	128.43
54	1w	55	PSU	N3-C2-N1	-8.57	121.62	128.43
54	2w	39	PSU	C2-N3-C4	8.55	122.36	115.14
54	1w	32	PSU	N3-C2-N1	-8.48	121.69	128.43
55	1x	55	PSU	N3-C2-N1	-8.43	121.73	128.43
54	2w	54	5MU	C2-N3-C4	8.42	122.25	115.14
1	1A	1917	PSU	N3-C2-N1	-8.39	121.76	128.43
1	1A	1911	PSU	N3-C2-N1	-8.39	121.76	128.43
54	2y	46	7MG	N3-C4-N9	8.33	137.60	126.91
1	1A	2605	PSU	N3-C2-N1	-8.23	121.89	128.43
32	1a	516	PSU	N3-C2-N1	-8.17	121.94	128.43
54	1y	39	PSU	N3-C2-N1	-8.11	121.98	128.43
55	1x	8	4SU	C4-N3-C2	8.02	126.78	115.15
55	2x	8	4SU	C4-N3-C2	7.94	126.66	115.15
54	1w	37	MIA	C12-C13-C14	-7.93	111.71	127.14
54	2y	54	5MU	C2-N3-C4	7.90	121.81	115.14
54	2w	46	7MG	N3-C4-N9	7.84	136.98	126.91
1	2A	2605	PSU	N3-C2-N1	-7.82	122.21	128.43
55	1x	54	5MU	C2-N3-C4	7.81	121.74	115.14
54	1y	39	PSU	C2-N3-C4	7.44	121.42	115.14
54	1y	55	PSU	C2-N3-C4	7.37	121.36	115.14
54	1w	55	PSU	C2-N3-C4	7.33	121.33	115.14
54	2y	32	PSU	C2-N3-C4	7.32	121.32	115.14
54	2y	39	PSU	N3-C2-N1	-7.31	122.62	128.43
54	1w	54	5MU	C2-N3-C4	7.22	121.24	115.14
54	1y	32	PSU	C2-N3-C4	7.21	121.23	115.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1911	PSU	C2-N3-C4	7.12	121.16	115.14
54	1w	39	PSU	C2-N3-C4	7.11	121.14	115.14
55	1x	55	PSU	C2-N3-C4	7.07	121.11	115.14
54	2w	55	PSU	C2-N3-C4	7.04	121.09	115.14
54	1w	32	PSU	C2-N3-C4	6.98	121.03	115.14
1	2A	1917	PSU	C2-N3-C4	6.93	121.00	115.14
55	2x	55	PSU	C2-N3-C4	6.90	120.97	115.14
1	1A	2503	2MA	C2-N3-C4	6.84	121.08	115.52
1	1A	1911	PSU	C2-N3-C4	6.77	120.86	115.14
32	2a	516	PSU	C2-N3-C4	6.77	120.86	115.14
32	1a	516	PSU	C2-N3-C4	6.68	120.78	115.14
54	2w	32	PSU	C2-N3-C4	6.67	120.78	115.14
54	2y	55	PSU	C2-N3-C4	6.65	120.76	115.14
1	1A	2605	PSU	C2-N3-C4	6.63	120.74	115.14
1	2A	1915	5MU	C2-N3-C4	6.54	120.67	115.14
1	1A	1917	PSU	C2-N3-C4	6.53	120.66	115.14
1	1A	1915	5MU	C2-N3-C4	6.42	120.56	115.14
1	1A	1939	5MU	C2-N3-C4	6.21	120.38	115.14
55	2x	54	5MU	C2-N3-C4	6.20	120.37	115.14
55	1x	55	PSU	C5-C4-N3	-5.89	117.77	125.36
54	1y	39	PSU	C5-C4-N3	-5.81	117.88	125.36
54	1w	46	7MG	N9-C8-N7	-5.79	95.09	103.38
54	2y	46	7MG	N9-C8-N7	-5.63	95.32	103.38
1	2A	2503	2MA	C2-N3-C4	5.59	120.06	115.52
54	2w	39	PSU	C5-C4-N3	-5.58	118.17	125.36
54	2w	46	7MG	N9-C8-N7	-5.57	95.41	103.38
54	1w	46	7MG	C2-N1-C6	5.53	124.71	115.93
54	1w	55	PSU	C5-C4-N3	-5.53	118.24	125.36
1	2A	1911	PSU	C5-C4-N3	-5.51	118.26	125.36
54	1y	55	PSU	C5-C4-N3	-5.49	118.29	125.36
54	1w	32	PSU	C5-C4-N3	-5.46	118.33	125.36
55	2x	55	PSU	C5-C4-N3	-5.45	118.33	125.36
1	2A	1917	PSU	C5-C4-N3	-5.45	118.34	125.36
54	1y	32	PSU	C5-C4-N3	-5.45	118.34	125.36
54	1w	39	PSU	C5-C4-N3	-5.44	118.35	125.36
54	1y	46	7MG	C5-C4-N3	-5.44	117.61	126.49
54	2w	55	PSU	C5-C4-N3	-5.39	118.42	125.36
32	2a	527	7MG	N9-C8-N7	-5.37	95.70	103.38
32	1a	527	7MG	C5-C4-N3	-5.35	117.75	126.49
54	2y	32	PSU	C5-C4-N3	-5.34	118.48	125.36
54	2w	32	PSU	C5-C4-N3	-5.34	118.49	125.36
1	1A	1911	PSU	C5-C4-N3	-5.31	118.52	125.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2y	55	PSU	C5-C4-N3	-5.26	118.58	125.36
1	2A	1939	5MU	C2-N3-C4	5.25	119.58	115.14
32	2a	516	PSU	C5-C4-N3	-5.25	118.60	125.36
54	2y	39	PSU	C2-N3-C4	5.24	119.56	115.14
32	1a	516	PSU	C5-C4-N3	-5.23	118.63	125.36
32	1a	966	M2G	C2-N1-C6	5.19	122.36	116.18
54	2y	46	7MG	C2-N1-C6	5.17	124.14	115.93
1	1A	2605	PSU	C5-C4-N3	-5.15	118.73	125.36
32	2a	1402	4OC	CM4-N4-C4	-5.14	118.56	122.97
1	1A	2251	OMG	C2-N3-C4	5.13	121.22	115.36
54	2y	39	PSU	C5-C4-N3	-5.10	118.79	125.36
1	1A	1920	4OC	C4-N3-C2	5.09	121.50	116.34
54	1y	39	PSU	O4'-C1'-C5	-5.06	102.10	109.93
1	1A	1917	PSU	C5-C4-N3	-5.01	118.90	125.36
32	2a	966	M2G	C2-N1-C6	4.98	122.12	116.18
32	2a	966	M2G	C2-N3-C4	4.97	120.92	115.28
32	2a	527	7MG	C5-C4-N3	-4.97	118.37	126.49
32	1a	527	7MG	N9-C8-N7	-4.86	96.42	103.38
54	1y	46	7MG	N9-C8-N7	-4.85	96.44	103.38
1	2A	2605	PSU	C5-C6-N1	-4.80	118.54	124.44
54	2w	8	4SU	C4-N3-C2	4.76	122.05	115.15
54	2w	46	7MG	C5-C4-N3	-4.75	118.73	126.49
1	2A	2251	OMG	C2-N3-C4	4.72	120.74	115.36
1	2A	2605	PSU	C2-N3-C4	4.71	119.12	115.14
1	1A	2605	PSU	C5-C6-N1	-4.70	118.66	124.44
54	1w	55	PSU	C5-C1'-C2'	-4.70	106.94	115.32
32	1a	1207	2MG	C2-N1-C6	4.69	123.59	115.18
1	2A	2503	2MA	C5-C6-N1	-4.62	118.21	123.06
1	1A	2251	OMG	C2-N1-C6	4.62	123.27	115.93
32	1a	1207	2MG	C5-C6-N1	-4.59	117.16	123.43
54	1w	8	4SU	C4-N3-C2	4.57	121.78	115.15
54	1y	46	7MG	C2-N1-C6	4.57	123.19	115.93
32	1a	1207	2MG	C2-N3-C4	4.55	120.44	115.28
1	1A	2503	2MA	C5-C6-N1	-4.54	118.29	123.06
54	1y	8	4SU	C4-N3-C2	4.54	121.74	115.15
32	1a	527	7MG	C4-C5-C6	4.53	120.06	115.20
55	2x	8	4SU	C5-C4-N3	-4.51	117.80	123.83
32	2a	1207	2MG	C5-C6-N1	-4.49	117.29	123.43
54	2y	46	7MG	C5-C4-N3	-4.45	119.22	126.49
32	1a	966	M2G	C5-C6-N1	-4.43	117.37	123.43
54	2w	32	PSU	C5-C6-N1	-4.42	119.01	124.44
1	2A	2605	PSU	C6-N1-C2	4.39	122.61	115.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1917	PSU	C5-C6-N1	-4.37	119.06	124.44
1	2A	1917	PSU	C6-N1-C2	4.36	122.55	115.36
54	1w	37	MIA	C2-N3-C4	4.35	121.32	115.32
1	2A	1920	4OC	C4-N3-C2	4.34	120.74	116.34
54	2w	32	PSU	C6-N1-C2	4.32	122.49	115.36
32	2a	527	7MG	C2-N1-C6	4.30	122.76	115.93
32	1a	1402	4OC	CM4-N4-C4	-4.29	119.28	122.97
54	2y	8	4SU	C4-N3-C2	4.29	121.37	115.15
1	1A	1911	PSU	C5-C6-N1	-4.24	119.23	124.44
32	1a	1207	2MG	C4-C5-C6	-4.24	116.75	120.80
54	2y	55	PSU	C6-N1-C2	4.23	122.34	115.36
55	1x	8	4SU	C5-C4-N3	-4.23	118.17	123.83
32	2a	1407	5MC	C4-N3-C2	4.21	121.10	116.02
1	2A	2605	PSU	C5-C4-N3	-4.19	119.97	125.36
54	2w	55	PSU	C5-C1'-C2'	-4.17	107.88	115.32
1	1A	2251	OMG	C5-C6-N1	-4.17	117.73	123.43
55	1x	55	PSU	C5-C6-N1	-4.16	119.32	124.44
54	1w	37	MIA	C15-C14-C13	-4.16	110.62	122.65
32	2a	1207	2MG	C4-C5-C6	-4.16	116.83	120.80
1	1A	1911	PSU	C6-N1-C2	4.16	122.22	115.36
1	1A	2605	PSU	C6-N1-C2	4.15	122.21	115.36
1	1A	1917	PSU	C5-C6-N1	-4.15	119.34	124.44
32	1a	527	7MG	C2-N1-C6	4.15	122.52	115.93
54	1y	46	7MG	C4-C5-C6	4.13	119.63	115.20
54	1y	32	PSU	C6-N1-C2	4.13	122.17	115.36
1	1A	1917	PSU	C6-N1-C2	4.12	122.15	115.36
32	1a	966	M2G	C2-N3-C4	4.11	119.95	115.28
55	2x	55	PSU	C6-N1-C2	4.11	122.14	115.36
54	2w	55	PSU	C6-N1-C2	4.11	122.14	115.36
54	1w	46	7MG	C5-C6-N1	-4.09	114.73	123.14
54	2y	32	PSU	C6-N1-C2	4.09	122.10	115.36
32	2a	966	M2G	C5-C6-N1	-4.08	117.85	123.43
32	2a	516	PSU	C6-N1-C2	4.08	122.09	115.36
55	2x	55	PSU	C5-C6-N1	-4.07	119.43	124.44
54	1w	32	PSU	C6-N1-C2	4.06	122.06	115.36
1	1A	2251	OMG	C4-C5-C6	-4.05	116.93	120.80
54	1w	46	7MG	C5-C4-N3	-4.05	119.89	126.49
32	2a	516	PSU	C5-C6-N1	-4.04	119.47	124.44
54	2y	55	PSU	C5-C6-N1	-4.04	119.48	124.44
54	1w	39	PSU	C6-N1-C2	4.02	122.00	115.36
32	1a	516	PSU	C6-N1-C2	4.01	121.97	115.36
32	2a	1400	5MC	C4-N3-C2	4.01	120.85	116.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2251	OMG	C2-N1-C6	3.98	122.25	115.93
32	1a	516	PSU	C5-C6-N1	-3.97	119.56	124.44
54	1w	39	PSU	C5-C6-N1	-3.96	119.57	124.44
55	1x	55	PSU	C6-N1-C2	3.96	121.89	115.36
32	2a	1207	2MG	C2-N3-C4	3.95	119.76	115.28
54	2y	39	PSU	C6-N1-C2	3.94	121.87	115.36
32	2a	1207	2MG	C2-N1-C6	3.94	122.23	115.18
54	2w	39	PSU	C6-N1-C2	3.91	121.82	115.36
54	1w	32	PSU	C5-C6-N1	-3.91	119.64	124.44
54	2w	55	PSU	C5-C6-N1	-3.88	119.67	124.44
54	1w	37	MIA	C16-C14-C13	-3.86	111.49	122.65
1	1A	2251	OMG	N3-C2-N1	-3.86	122.08	127.22
55	2x	32	5MC	C4-N3-C2	3.82	120.63	116.02
1	2A	1911	PSU	C6-N1-C2	3.82	121.66	115.36
1	1A	1942	5MC	C4-N3-C2	3.80	120.61	116.02
32	1a	1404	5MC	C4-N3-C2	3.80	120.60	116.02
1	2A	1917	PSU	C5-C1'-C2'	-3.77	108.59	115.32
32	2a	527	7MG	C4-C5-C6	3.77	119.24	115.20
32	2a	967	5MC	C4-N3-C2	3.74	120.53	116.02
32	1a	967	5MC	C4-N3-C2	3.72	120.51	116.02
32	2a	966	M2G	C4-C5-C6	-3.71	117.25	120.80
54	2w	32	PSU	C5-C1'-C2'	-3.71	108.70	115.32
1	2A	2251	OMG	C5-C6-N1	-3.70	118.37	123.43
54	2w	46	7MG	C2-N1-C6	3.69	121.80	115.93
54	1w	55	PSU	C6-N1-C2	3.69	121.44	115.36
1	2A	1942	5MC	C4-N3-C2	3.66	120.44	116.02
1	2A	1939	5MU	C5-C6-N1	-3.66	118.25	122.19
32	2a	1518	MA6	C9-N6-C6	-3.66	108.44	119.51
1	2A	1911	PSU	C5-C6-N1	-3.66	119.95	124.44
54	1y	32	PSU	C5-C6-N1	-3.64	119.96	124.44
32	1a	1518	MA6	N3-C2-N1	-3.62	123.01	128.68
32	1a	527	7MG	C5-C6-N1	-3.62	115.70	123.14
32	2a	1518	MA6	C4-C5-N7	-3.62	105.63	109.40
54	2y	32	PSU	C5-C6-N1	-3.61	120.00	124.44
32	2a	1519	MA6	C4-C5-N7	-3.61	105.64	109.40
1	2A	2251	OMG	C4-C5-C6	-3.58	117.38	120.80
1	1A	1962	5MC	C4-N3-C2	3.58	120.34	116.02
54	1y	46	7MG	C5-C6-N1	-3.58	115.79	123.14
32	1a	1519	MA6	N3-C2-N1	-3.56	123.12	128.68
54	2y	46	7MG	C5-C6-N1	-3.55	115.85	123.14
54	1w	46	7MG	C4-C5-C6	3.54	119.00	115.20
54	2w	46	7MG	C4-C5-C6	3.54	119.00	115.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1y	55	PSU	C6-N1-C2	3.54	121.20	115.36
32	2a	1518	MA6	N3-C2-N1	-3.51	123.19	128.68
1	1A	1917	PSU	C5-C1'-C2'	-3.51	109.06	115.32
32	1a	1407	5MC	C4-N3-C2	3.48	120.22	116.02
32	1a	966	M2G	C4-C5-C6	-3.48	117.47	120.80
54	2w	39	PSU	C5-C6-N1	-3.47	120.17	124.44
54	1y	37	MIA	N3-C2-N1	-3.46	123.27	128.68
54	1w	37	MIA	C5-C6-N1	-3.46	117.94	120.81
32	2a	1207	2MG	C4-C5-N7	-3.45	105.80	109.40
32	2a	527	7MG	C5-C6-N1	-3.45	116.04	123.14
32	1a	1400	5MC	C4-N3-C2	3.45	120.18	116.02
1	2A	1962	5MC	C4-N3-C2	3.44	120.17	116.02
54	1y	39	PSU	C6-N1-C2	3.42	121.00	115.36
1	1A	1911	PSU	C5-C1'-C2'	-3.41	109.23	115.32
55	1x	55	PSU	C5-C1'-C2'	-3.40	109.25	115.32
54	2y	39	PSU	C5-C6-N1	-3.39	120.27	124.44
54	2y	37	MIA	N3-C2-N1	-3.36	123.42	128.68
54	2w	46	7MG	C5-C6-N1	-3.36	116.23	123.14
54	2w	37	MIA	N3-C2-N1	-3.36	123.43	128.68
54	2w	8	4SU	C5-C4-N3	-3.34	119.36	123.83
32	1a	1519	MA6	C4-C5-N7	-3.34	105.91	109.40
32	2a	1404	5MC	C4-N3-C2	3.29	119.99	116.02
1	1A	1942	5MC	N4-C4-N3	3.29	121.68	117.03
32	2a	1519	MA6	C9-N6-C6	-3.28	109.57	119.51
55	1x	32	5MC	C4-N3-C2	3.28	119.98	116.02
32	1a	1207	2MG	C4-C5-N7	-3.25	106.02	109.40
32	2a	1519	MA6	N3-C2-N1	-3.23	123.63	128.68
1	2A	2251	OMG	N3-C2-N1	-3.23	122.92	127.22
1	2A	1962	5MC	N4-C4-N3	3.22	121.59	117.03
32	1a	1519	MA6	C9-N6-C6	-3.18	109.87	119.51
32	1a	1518	MA6	C4-C5-N7	-3.16	106.10	109.40
1	1A	2251	OMG	C4-C5-N7	-3.15	106.11	109.40
32	2a	1207	2MG	CM2-N2-C2	-3.13	119.81	123.59
1	1A	1939	5MU	C5-C6-N1	-3.13	118.83	122.19
54	1w	46	7MG	C5-C4-N9	-3.09	102.11	106.44
54	1w	8	4SU	C5-C4-N3	-3.08	119.71	123.83
54	1w	55	PSU	C5-C6-N1	-3.01	120.73	124.44
1	1A	2605	PSU	C5-C1'-C2'	-3.00	109.97	115.32
32	1a	1518	MA6	C9-N6-C6	-2.96	110.56	119.51
54	1w	39	PSU	C5-C1'-C2'	-2.92	110.11	115.32
32	2a	1400	5MC	N4-C4-N3	2.92	121.16	117.03
54	2y	46	7MG	C4-C5-C6	2.92	118.33	115.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1207	2MG	CM2-N2-C2	-2.92	120.07	123.59
54	1y	37	MIA	C4-C5-N7	-2.91	106.36	109.40
54	2y	39	PSU	O4'-C1'-C5	-2.91	105.43	109.93
32	1a	966	M2G	CM2-N2-C2	-2.86	118.56	121.29
54	1y	39	PSU	C5-C6-N1	-2.86	120.92	124.44
54	1y	8	4SU	C5-C4-N3	-2.84	120.03	123.83
55	1x	32	5MC	C5-C6-N1	-2.82	119.15	122.19
32	2a	1407	5MC	N4-C4-N3	2.80	121.00	117.03
54	2w	46	7MG	C8-N7-C5	2.79	116.20	108.94
32	2a	527	7MG	C8-N7-C5	2.75	116.08	108.94
32	1a	966	M2G	C4-C5-N7	-2.74	106.54	109.40
32	2a	966	M2G	C4-C5-N7	-2.73	106.55	109.40
54	2y	8	4SU	C5-C4-N3	-2.73	120.18	123.83
54	1w	37	MIA	C4-C5-N7	-2.72	106.56	109.40
54	2y	46	7MG	C8-N7-C5	2.72	116.01	108.94
54	2y	39	PSU	C5-C1'-C2'	-2.70	110.50	115.32
54	2y	37	MIA	C4-C5-N7	-2.70	106.58	109.40
32	2a	1207	2MG	N2-C2-N1	2.70	119.55	116.96
54	1w	37	MIA	C2-N1-C6	2.70	122.02	117.19
54	2w	37	MIA	C4-C5-N7	-2.65	106.64	109.40
32	1a	527	7MG	C8-N7-C5	2.64	115.80	108.94
54	1y	55	PSU	C5-C6-N1	-2.63	121.20	124.44
1	2A	1915	5MU	C5-C6-N1	-2.63	119.36	122.19
54	1y	46	7MG	C8-N7-C5	2.63	115.77	108.94
32	1a	1498	UR3	C3U-N3-C4	2.57	121.53	118.12
32	1a	1407	5MC	N4-C4-N3	2.56	120.65	117.03
32	2a	967	5MC	C5-C6-N1	-2.55	119.44	122.19
32	1a	1518	MA6	N1-C6-N6	2.55	119.74	117.06
54	1w	46	7MG	C8-N7-C5	2.54	115.55	108.94
54	2y	55	PSU	C5-C1'-C2'	-2.54	110.79	115.32
32	1a	1404	5MC	N4-C4-N3	2.53	120.61	117.03
1	2A	2503	2MA	C4-C5-N7	-2.52	106.77	109.40
1	2A	1942	5MC	N4-C4-N3	2.50	120.57	117.03
55	1x	32	5MC	N4-C4-N3	2.50	120.56	117.03
32	2a	1518	MA6	C10-N6-C9	-2.49	108.11	116.12
1	2A	1942	5MC	C5-C6-N1	-2.48	119.53	122.19
1	2A	1911	PSU	C5-C1'-C2'	-2.47	110.91	115.32
1	1A	1962	5MC	N4-C4-N3	2.46	120.51	117.03
55	2x	32	5MC	N4-C4-N3	2.44	120.49	117.03
1	1A	1920	4OC	N4-C4-N3	2.44	120.34	116.49
32	1a	1207	2MG	N3-C2-N1	-2.41	122.41	126.23
54	1w	37	MIA	N3-C2-N1	-2.37	122.62	126.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1404	5MC	N4-C4-N3	2.36	120.37	117.03
54	2y	46	7MG	C2-N3-C4	2.36	120.42	113.89
32	1a	967	5MC	C5-C6-N1	-2.35	119.66	122.19
54	2y	46	7MG	C5-C4-N9	-2.35	103.16	106.44
32	2a	1207	2MG	C1'-N9-C4	-2.34	122.52	126.64
32	2a	1404	5MC	C5-C6-N1	-2.33	119.68	122.19
54	1y	46	7MG	C2-N3-C4	2.32	120.31	113.89
32	2a	967	5MC	N4-C4-N3	2.32	120.32	117.03
55	2x	54	5MU	C5-C6-N1	-2.32	119.69	122.19
32	1a	1400	5MC	C5-C6-N1	-2.29	119.72	122.19
1	2A	2605	PSU	C5-C1'-C2'	-2.29	111.23	115.32
32	1a	967	5MC	N4-C4-N3	2.29	120.27	117.03
55	1x	54	5MU	C5-C6-N1	-2.28	119.74	122.19
32	2a	1498	UR3	C3U-N3-C4	2.25	121.10	118.12
32	1a	1400	5MC	N4-C4-N3	2.24	120.20	117.03
32	1a	516	PSU	O4'-C1'-C2'	2.22	108.26	104.66
32	2a	516	PSU	O4'-C1'-C2'	2.22	108.26	104.66
54	2w	46	7MG	C2-N3-C4	2.22	120.03	113.89
1	2A	1962	5MC	C5-C6-N1	-2.22	119.81	122.19
54	2y	46	7MG	N2-C2-N1	2.18	120.64	117.25
1	2A	1920	4OC	N4-C4-N3	2.18	119.94	116.49
32	1a	1404	5MC	C5-C6-N1	-2.18	119.85	122.19
1	2A	2251	OMG	C4-C5-N7	-2.18	107.13	109.40
54	1w	54	5MU	C5-C6-N1	-2.18	119.85	122.19
32	2a	527	7MG	C5-C4-N9	-2.17	103.40	106.44
32	1a	1518	MA6	C10-N6-C9	-2.17	109.13	116.12
1	1A	1962	5MC	C5-C6-N1	-2.17	119.86	122.19
1	1A	1920	4OC	CM2-O2'-C2'	-2.17	108.84	114.52
32	1a	527	7MG	C5-C4-N9	-2.17	103.41	106.44
54	2y	46	7MG	N3-C2-N1	-2.16	122.03	125.42
1	1A	2503	2MA	C4-C5-N7	-2.15	107.15	109.40
54	2y	46	7MG	O4'-C1'-N9	-2.12	106.49	109.35
1	1A	2552	2MU	C5-C4-N3	-2.11	118.66	123.31
54	2y	46	7MG	CM7-N7-C5	2.11	132.11	124.01
32	1a	1207	2MG	C1'-N9-C4	-2.09	122.97	126.64
54	2w	46	7MG	N2-C2-N1	2.09	120.50	117.25
32	1a	527	7MG	CM7-N7-C5	2.08	132.00	124.01
1	2A	2552	2MU	C5-C4-N3	-2.07	118.75	123.31
32	1a	527	7MG	C2-N3-C4	2.07	119.61	113.89
1	1A	1942	5MC	C5-C6-N1	-2.07	119.97	122.19
32	2a	527	7MG	C2-N3-C4	2.06	119.60	113.89
1	1A	1915	5MU	C5-C6-N1	-2.05	119.99	122.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1w	46	7MG	CM7-N7-C5	2.04	131.84	124.01
32	1a	1207	2MG	N2-C2-N1	2.03	118.91	116.96
1	2A	2503	2MA	C1'-N9-C4	-2.03	123.08	126.64
54	2y	39	PSU	C1'-C5-C4	2.02	124.92	121.12
54	1y	46	7MG	C5-C4-N9	-2.01	103.62	106.44
32	1a	1519	MA6	C1'-N9-C4	-2.01	123.11	126.64

There are no chirality outliers.

All (79) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1A	1920	4OC	C2'-C1'-N1-C6
1	2A	1939	5MU	C2'-C1'-N1-C6
1	2A	1939	5MU	O4'-C1'-N1-C6
1	1A	1962	5MC	O4'-C1'-N1-C6
1	1A	1962	5MC	C2'-C1'-N1-C6
1	2A	1962	5MC	O4'-C1'-N1-C6
1	2A	1962	5MC	C2'-C1'-N1-C6
32	1a	1207	2MG	N1-C2-N2-CM2
32	1a	1207	2MG	N3-C2-N2-CM2
32	2a	1400	5MC	C4'-C5'-O5'-P
32	2a	1402	4OC	C2'-C1'-N1-C6
32	1a	1518	MA6	C5-C6-N6-C10
32	2a	1518	MA6	C5-C6-N6-C9
32	2a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
32	2a	1519	MA6	C5-C6-N6-C10
43	1l	92	0TD	CG-CB-SB-CSB
43	2l	92	0TD	O-C-CA-CB
43	2l	92	0TD	CG-CB-SB-CSB
54	2y	8	4SU	C2'-C1'-N1-C6
54	1w	37	MIA	C12-C13-C14-C16
54	1y	39	PSU	C3'-C4'-C5'-O5'
54	2y	39	PSU	C3'-C4'-C5'-O5'
54	1w	46	7MG	C4'-C5'-O5'-P
54	1y	46	7MG	C4'-C5'-O5'-P
55	2x	8	4SU	C2'-C1'-N1-C6
55	2x	32	5MC	O4'-C1'-N1-C6
55	2x	32	5MC	C2'-C1'-N1-C6
32	1a	527	7MG	C3'-C4'-C5'-O5'
32	2a	1402	4OC	O4'-C4'-C5'-O5'
32	1a	1519	MA6	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
54	2y	46	7MG	O4'-C4'-C5'-O5'
32	2a	967	5MC	O4'-C4'-C5'-O5'
32	1a	1402	4OC	O4'-C4'-C5'-O5'
32	2a	1402	4OC	C3'-C4'-C5'-O5'
54	1y	39	PSU	O4'-C4'-C5'-O5'
54	2y	39	PSU	O4'-C4'-C5'-O5'
54	2y	46	7MG	C3'-C4'-C5'-O5'
32	2a	1518	MA6	N1-C6-N6-C9
54	2y	37	MIA	C3'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
54	1y	46	7MG	C3'-C4'-C5'-O5'
32	1a	527	7MG	O4'-C4'-C5'-O5'
32	1a	1402	4OC	C3'-C4'-C5'-O5'
54	2y	37	MIA	O4'-C4'-C5'-O5'
54	2w	46	7MG	C2'-C1'-N9-C8
32	1a	1519	MA6	C5-C6-N6-C10
32	2a	1519	MA6	C5-C6-N6-C9
54	1y	46	7MG	C2'-C1'-N9-C8
32	2a	1519	MA6	C4'-C5'-O5'-P
54	1w	37	MIA	N1-C2-S10-C11
1	1A	1915	5MU	O4'-C4'-C5'-O5'
54	2y	46	7MG	C2'-C1'-N9-C8
32	2a	527	7MG	C4'-C5'-O5'-P
32	2a	1518	MA6	C5-C6-N6-C10
54	2y	55	PSU	C3'-C4'-C5'-O5'
54	1w	37	MIA	N3-C2-S10-C11
32	1a	527	7MG	C4'-C5'-O5'-P
32	2a	1519	MA6	N1-C6-N6-C9
32	2a	967	5MC	C3'-C4'-C5'-O5'
54	1y	46	7MG	C2'-C1'-N9-C4
54	2w	46	7MG	C2'-C1'-N9-C4
54	1y	46	7MG	O4'-C1'-N9-C8
54	2y	46	7MG	O4'-C1'-N9-C8
54	2y	55	PSU	O4'-C1'-C5-C4
43	1l	92	0TD	CA-CB-SB-CSB
43	2l	92	0TD	CA-CB-SB-CSB
32	1a	1400	5MC	O4'-C4'-C5'-O5'
54	1w	32	PSU	C2'-C1'-C5-C6
54	1y	46	7MG	O4'-C4'-C5'-O5'
32	1a	1519	MA6	C4'-C5'-O5'-P
1	2A	2251	OMG	C4'-C5'-O5'-P
1	1A	2503	2MA	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
54	2y	46	7MG	C2'-C1'-N9-C4
32	1a	1402	4OC	C3'-C2'-O2'-CM2
1	1A	1915	5MU	C3'-C4'-C5'-O5'
1	1A	2503	2MA	O4'-C4'-C5'-O5'
1	2A	2503	2MA	O4'-C4'-C5'-O5'
32	1a	1400	5MC	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2321 ligands modelled in this entry, 2315 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
60	SF4	2d	301	35	0,12,12	-	-	-		
60	SF4	1d	501	35	0,12,12	-	-	-		
58	HGR	1A	3915	56	39,39,39	2.40	8 (20%)	50,58,58	1.81	13 (26%)
61	FME	1x	3011	55	8,9,10	0.39	0	7,9,11	1.35	1 (14%)
58	HGR	2A	3652	-	39,39,39	2.39	8 (20%)	50,58,58	1.71	13 (26%)
61	FME	2x	103	55	8,9,10	0.48	0	7,9,11	1.29	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	SF4	2d	301	35	-	-	0/6/5/5
60	SF4	1d	501	35	-	-	0/6/5/5
58	HGR	1A	3915	56	-	6/20/79/79	0/4/4/4
61	FME	1x	3011	55	-	5/7/9/11	-
58	HGR	2A	3652	-	-	6/20/79/79	0/4/4/4
61	FME	2x	103	55	-	5/7/9/11	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	2A	3652	HGR	C12-C14	9.34	1.55	1.33
58	1A	3915	HGR	C12-C14	8.89	1.54	1.33
58	1A	3915	HGR	C5-C6	-5.35	1.39	1.50
58	2A	3652	HGR	C5-C4	-5.31	1.39	1.49
58	2A	3652	HGR	C5-C6	-5.29	1.39	1.50
58	1A	3915	HGR	C5-C4	-5.22	1.39	1.49
58	1A	3915	HGR	C3-C2	-4.67	1.39	1.48
58	2A	3652	HGR	C3-C2	-4.65	1.39	1.48
58	1A	3915	HGR	O4-C2	4.60	1.36	1.24
58	2A	3652	HGR	O4-C2	4.31	1.36	1.24
58	1A	3915	HGR	C1-C6	2.78	1.39	1.35
58	2A	3652	HGR	C1-C6	2.77	1.39	1.35
58	1A	3915	HGR	O8-C23	2.46	1.45	1.41
58	2A	3652	HGR	O8-C23	2.20	1.45	1.41
58	2A	3652	HGR	O9-C23	2.04	1.44	1.41
58	1A	3915	HGR	C1-C2	-2.03	1.39	1.44

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	1A	3915	HGR	C12-C6-C1	-4.71	114.97	119.31
58	2A	3652	HGR	C10-C9-C8	-4.57	96.50	102.30
58	2A	3652	HGR	C4-C5-C6	4.33	121.68	112.36
58	1A	3915	HGR	C23-O9-C22	-4.22	99.88	106.31
58	1A	3915	HGR	C4-C5-C6	3.84	120.63	112.36
58	1A	3915	HGR	C10-C9-C8	-3.63	97.70	102.30
58	1A	3915	HGR	O8-C18-C22	-3.53	98.05	105.97
58	2A	3652	HGR	C12-C6-C1	-3.40	116.18	119.31
58	1A	3915	HGR	O9-C22-C18	-3.26	98.67	105.97
58	1A	3915	HGR	C4-C3-C2	-3.16	118.92	121.83
58	2A	3652	HGR	C9-C8-C7	-3.15	97.96	101.64
58	2A	3652	HGR	O9-C22-C18	-3.00	99.26	105.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	2A	3652	HGR	O4-C2-C3	-2.89	116.77	121.30
58	2A	3652	HGR	C23-O9-C22	-2.81	102.03	106.31
58	1A	3915	HGR	C8-C7-C11	-2.78	108.79	113.67
58	2A	3652	HGR	O8-C18-C22	-2.71	99.89	105.97
58	1A	3915	HGR	O1-C10-C9	-2.49	101.77	104.98
58	2A	3652	HGR	C1-C2-C3	2.35	120.52	115.99
58	2A	3652	HGR	C4-C3-C2	-2.34	119.68	121.83
58	1A	3915	HGR	O4-C2-C3	-2.29	117.72	121.30
58	1A	3915	HGR	O3-C3-C2	2.24	116.82	112.56
58	2A	3652	HGR	C8-C7-C11	-2.23	109.76	113.67
58	1A	3915	HGR	C1-C2-C3	2.22	120.28	115.99
58	2A	3652	HGR	C19-C17-N1	2.20	114.76	110.62
58	1A	3915	HGR	C9-C8-C7	-2.13	99.16	101.64
61	1x	3011	FME	CA-N-CN	-2.12	119.56	122.82
58	2A	3652	HGR	O3-C3-C2	2.08	116.53	112.56
61	2x	103	FME	CA-N-CN	-2.08	119.63	122.82

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	1A	3915	HGR	C2-C3-O3-C10
58	2A	3652	HGR	C2-C3-O3-C10
61	1x	3011	FME	O1-CN-N-CA
61	1x	3011	FME	N-CA-CB-CG
61	1x	3011	FME	C-CA-CB-CG
61	1x	3011	FME	O-C-CA-CB
61	1x	3011	FME	CA-CB-CG-SD
61	2x	103	FME	O1-CN-N-CA
61	2x	103	FME	C-CA-CB-CG
61	2x	103	FME	O-C-CA-CB
61	2x	103	FME	CA-CB-CG-SD
61	2x	103	FME	N-CA-CB-CG
58	1A	3915	HGR	C12-C14-C15-O7
58	1A	3915	HGR	C12-C14-C15-N1
58	2A	3652	HGR	C12-C14-C15-O7
58	2A	3652	HGR	C12-C14-C15-N1
58	1A	3915	HGR	C16-C14-C15-O7
58	1A	3915	HGR	C16-C14-C15-N1
58	2A	3652	HGR	C16-C14-C15-O7
58	2A	3652	HGR	C16-C14-C15-N1
58	1A	3915	HGR	C19-C17-N1-C15

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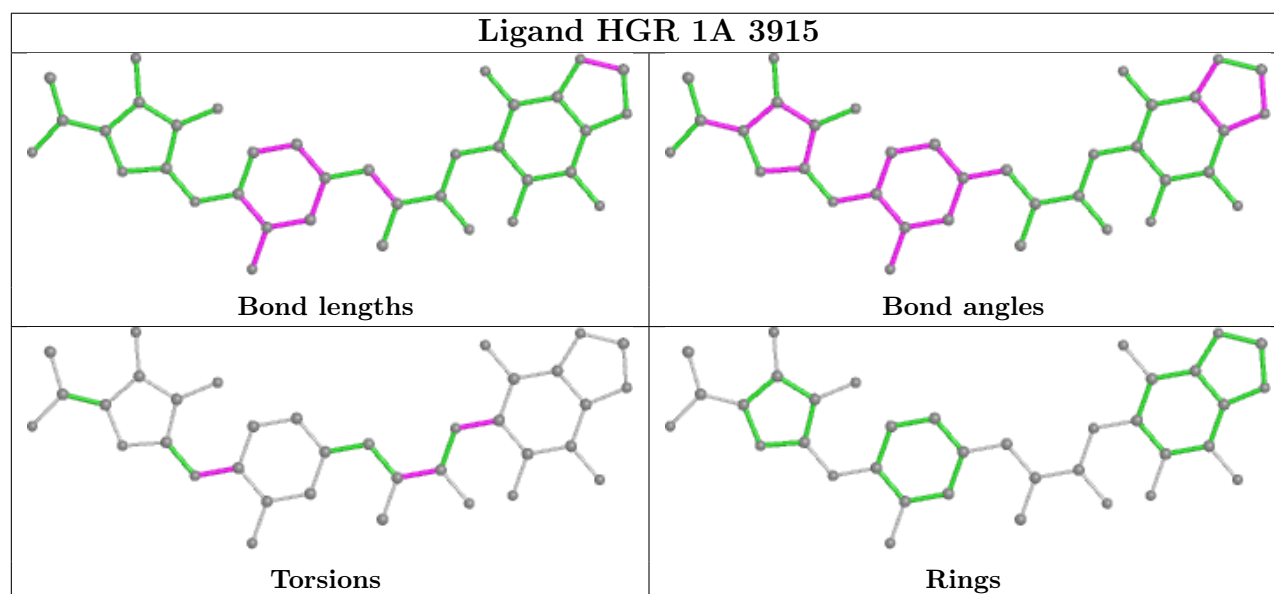
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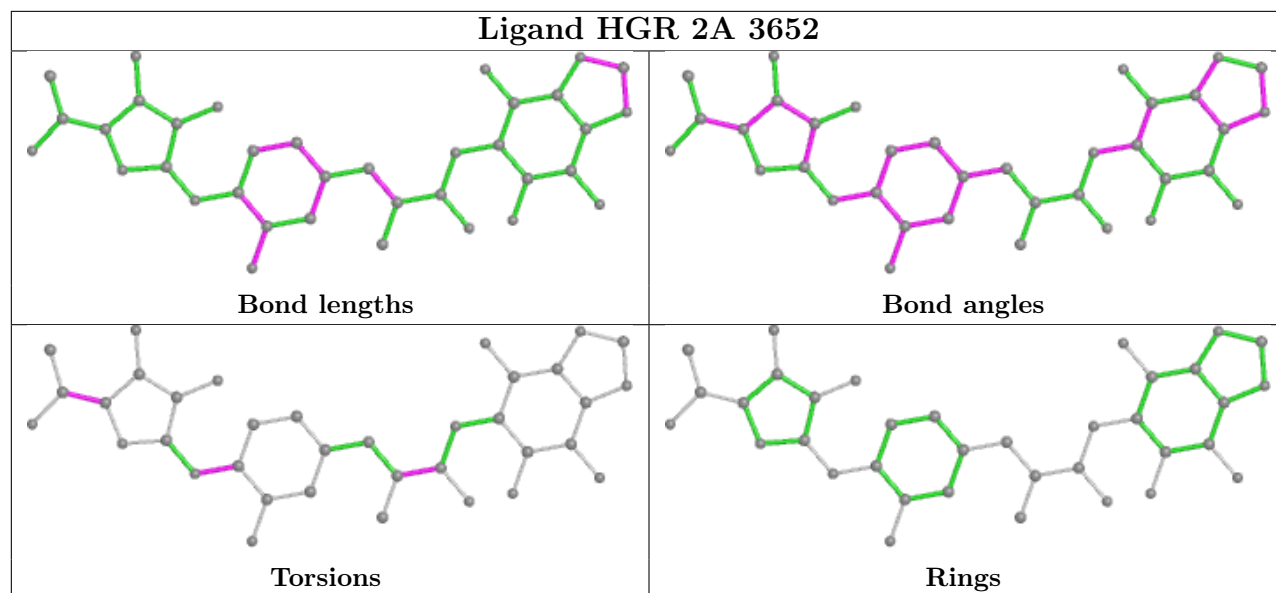
Mol	Chain	Res	Type	Atoms
58	2A	3652	HGR	O6-C11-C7-O1

There are no ring outliers.

No monomer is involved in short contacts.

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1A	2860/2915 (98%)	0.56	46 (1%) 72 68	22, 42, 90, 106	0
1	2A	2789/2915 (95%)	0.05	51 (1%) 68 64	26, 45, 87, 104	0
2	1B	120/121 (99%)	0.36	0 100 100	37, 58, 69, 86	0
2	2B	120/121 (99%)	-0.02	2 (1%) 70 66	44, 65, 74, 87	0
3	1D	275/276 (99%)	0.83	10 (3%) 42 35	21, 41, 58, 73	0
3	2D	275/276 (99%)	0.50	9 (3%) 46 39	25, 42, 61, 72	0
4	1E	204/206 (99%)	0.63	2 (0%) 82 80	22, 46, 65, 78	0
4	2E	204/206 (99%)	0.40	4 (1%) 65 60	25, 49, 66, 79	0
5	1F	203/210 (96%)	0.55	3 (1%) 73 70	21, 50, 72, 83	0
5	2F	203/210 (96%)	0.41	6 (2%) 50 43	24, 54, 74, 85	0
6	1G	181/182 (99%)	0.67	9 (4%) 28 23	49, 66, 77, 91	0
6	2G	181/182 (99%)	1.04	34 (18%) 1 0	53, 69, 80, 93	0
7	1H	174/180 (96%)	0.63	3 (1%) 70 66	47, 63, 73, 81	0
7	2H	174/180 (96%)	0.97	25 (14%) 2 1	53, 67, 76, 82	0
8	1I	146/148 (98%)	0.13	1 (0%) 87 86	44, 72, 81, 85	0
8	2I	146/148 (98%)	0.04	1 (0%) 87 86	47, 72, 81, 84	0
9	1N	140/140 (100%)	0.42	0 100 100	23, 37, 59, 69	0
9	2N	140/140 (100%)	1.31	30 (21%) 0 0	37, 64, 76, 84	0
10	1O	122/122 (100%)	0.68	4 (3%) 46 39	26, 39, 58, 66	0
10	2O	122/122 (100%)	0.95	15 (12%) 4 2	39, 56, 68, 78	0
11	1P	149/150 (99%)	0.66	4 (2%) 54 48	22, 52, 71, 81	0
11	2P	149/150 (99%)	0.28	4 (2%) 54 48	27, 55, 77, 82	0
12	1Q	141/141 (100%)	0.95	9 (6%) 19 14	32, 49, 63, 76	0
12	2Q	141/141 (100%)	1.80	52 (36%) 0 0	36, 53, 66, 77	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	0.65	3 (2%) 57 51	28, 39, 54, 64	0
13	2R	118/118 (100%)	0.33	1 (0%) 86 84	31, 41, 57, 64	0
14	1S	110/112 (98%)	0.60	1 (0%) 84 82	46, 58, 70, 74	0
14	2S	110/112 (98%)	0.50	9 (8%) 11 8	51, 61, 73, 77	0
15	1T	131/146 (89%)	0.63	2 (1%) 73 70	39, 51, 69, 75	0
15	2T	131/146 (89%)	0.31	1 (0%) 86 84	41, 53, 70, 74	0
16	1U	116/118 (98%)	0.67	4 (3%) 45 38	26, 39, 57, 71	0
16	2U	116/118 (98%)	0.48	4 (3%) 45 38	29, 44, 63, 72	0
17	1V	101/101 (100%)	0.46	0 100 100	26, 49, 66, 70	0
17	2V	101/101 (100%)	0.49	4 (3%) 38 31	30, 54, 69, 73	0
18	1W	112/113 (99%)	0.53	0 100 100	26, 36, 55, 83	0
18	2W	112/113 (99%)	0.49	2 (1%) 68 64	29, 39, 59, 86	0
19	1X	95/96 (98%)	0.63	0 100 100	30, 43, 63, 80	0
19	2X	95/96 (98%)	0.45	5 (5%) 26 20	34, 47, 65, 80	0
20	1Y	107/110 (97%)	0.47	0 100 100	44, 55, 71, 79	0
20	2Y	107/110 (97%)	0.80	12 (11%) 5 3	49, 59, 73, 81	0
21	1Z	154/206 (74%)	1.01	26 (16%) 1 1	37, 61, 82, 94	0
21	2Z	160/206 (77%)	1.69	56 (35%) 0 0	65, 80, 91, 97	0
22	10	83/85 (97%)	1.02	7 (8%) 11 7	24, 36, 65, 88	0
22	20	83/85 (97%)	1.28	13 (15%) 2 1	48, 64, 80, 89	0
23	11	97/98 (98%)	0.57	4 (4%) 37 30	23, 43, 67, 74	0
23	21	97/98 (98%)	0.54	5 (5%) 27 21	35, 55, 72, 76	0
24	12	70/72 (97%)	0.40	0 100 100	41, 56, 65, 68	0
24	22	70/72 (97%)	-0.02	0 100 100	45, 59, 68, 78	0
25	13	59/60 (98%)	0.45	0 100 100	28, 44, 65, 72	0
25	23	59/60 (98%)	1.51	15 (25%) 0 0	36, 49, 69, 76	0
26	14	69/71 (97%)	0.35	1 (1%) 75 71	49, 71, 85, 89	0
26	24	69/71 (97%)	1.26	16 (23%) 0 0	72, 83, 93, 97	0
27	15	59/60 (98%)	0.47	2 (3%) 45 38	17, 28, 46, 72	0
27	25	59/60 (98%)	0.44	1 (1%) 70 66	32, 49, 63, 72	0
28	16	53/54 (98%)	0.56	1 (1%) 66 62	33, 47, 60, 64	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.55	6 (11%) 5 3	35, 51, 61, 67	0
29	17	48/49 (97%)	0.68	4 (8%) 11 8	16, 25, 49, 72	0
29	27	48/49 (97%)	0.70	4 (8%) 11 8	31, 38, 63, 69	0
30	18	64/65 (98%)	0.63	0 100 100	32, 40, 49, 60	0
30	28	64/65 (98%)	0.48	0 100 100	36, 44, 52, 61	0
31	19	37/37 (100%)	1.01	4 (10%) 5 3	36, 47, 61, 70	0
31	29	37/37 (100%)	1.33	11 (29%) 0 0	42, 52, 64, 74	0
32	1a	1488/1521 (97%)	0.21	19 (1%) 77 73	39, 70, 90, 105	0
32	2a	1491/1521 (98%)	0.02	21 (1%) 75 71	42, 72, 91, 104	0
33	1b	231/256 (90%)	0.14	1 (0%) 92 91	67, 79, 88, 92	0
33	2b	231/256 (90%)	0.84	32 (13%) 2 1	67, 81, 88, 93	0
34	1c	206/239 (86%)	0.85	21 (10%) 6 4	66, 76, 83, 92	0
34	2c	206/239 (86%)	1.54	66 (32%) 0 0	69, 78, 85, 92	0
35	1d	208/209 (99%)	0.95	29 (13%) 2 1	57, 71, 79, 84	0
35	2d	208/209 (99%)	1.51	62 (29%) 0 0	58, 71, 79, 84	0
36	1e	148/162 (91%)	0.76	8 (5%) 25 20	48, 63, 73, 83	0
36	2e	148/162 (91%)	1.34	38 (25%) 0 0	67, 78, 85, 90	0
37	1f	100/101 (99%)	0.71	8 (8%) 12 9	46, 65, 74, 76	0
37	2f	100/101 (99%)	0.26	1 (1%) 82 80	55, 70, 79, 87	0
38	1g	155/156 (99%)	0.80	18 (11%) 4 3	61, 72, 81, 88	0
38	2g	155/156 (99%)	0.66	19 (12%) 4 2	64, 74, 82, 87	0
39	1h	137/138 (99%)	0.29	5 (3%) 42 35	52, 64, 73, 86	0
39	2h	137/138 (99%)	1.05	26 (18%) 1 0	60, 77, 84, 89	0
40	1i	127/128 (99%)	0.44	8 (6%) 20 15	59, 77, 85, 88	0
40	2i	127/128 (99%)	1.27	30 (23%) 0 0	64, 79, 86, 89	0
41	1j	97/105 (92%)	0.45	5 (5%) 27 21	56, 75, 85, 92	0
41	2j	96/105 (91%)	1.46	31 (32%) 0 0	68, 85, 92, 94	0
42	1k	114/129 (88%)	1.56	35 (30%) 0 0	37, 64, 73, 77	0
42	2k	114/129 (88%)	1.18	18 (15%) 2 1	44, 73, 81, 85	0
43	1l	121/132 (91%)	0.56	5 (4%) 37 30	41, 55, 68, 75	0
43	2l	121/132 (91%)	1.34	34 (28%) 0 0	50, 70, 79, 83	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	123/126 (97%)	0.91	13 (10%) 6 4	58, 73, 81, 84	0
44	2m	122/126 (96%)	1.47	35 (28%) 0 0	63, 76, 82, 85	0
45	1n	60/61 (98%)	1.05	6 (10%) 7 4	55, 64, 74, 80	0
45	2n	60/61 (98%)	3.62	49 (81%) 0 0	73, 85, 90, 94	0
46	1o	88/89 (98%)	0.96	13 (14%) 2 1	52, 66, 76, 83	0
46	2o	88/89 (98%)	0.21	2 (2%) 60 54	56, 68, 78, 85	0
47	1p	82/88 (93%)	0.73	6 (7%) 15 11	56, 68, 76, 81	0
47	2p	82/88 (93%)	0.79	4 (4%) 29 23	58, 68, 76, 82	0
48	1q	99/105 (94%)	0.65	4 (4%) 38 31	59, 68, 76, 78	0
48	2q	99/105 (94%)	0.89	17 (17%) 1 0	60, 69, 77, 80	0
49	1r	68/88 (77%)	0.84	8 (11%) 4 3	57, 67, 76, 82	0
49	2r	68/88 (77%)	0.33	4 (5%) 22 17	57, 68, 77, 83	0
50	1s	83/93 (89%)	0.66	6 (7%) 15 11	64, 76, 84, 91	0
50	2s	83/93 (89%)	2.09	41 (49%) 0 0	67, 79, 86, 93	0
51	1t	96/106 (90%)	0.45	3 (3%) 49 42	56, 67, 77, 81	0
51	2t	96/106 (90%)	0.26	2 (2%) 63 58	56, 68, 78, 80	0
52	1u	23/27 (85%)	0.89	4 (17%) 1 0	62, 70, 74, 75	0
52	2u	23/27 (85%)	1.22	6 (26%) 0 0	65, 72, 76, 76	0
53	1v	14/27 (51%)	2.03	7 (50%) 0 0	55, 73, 97, 105	0
53	2v	13/27 (48%)	2.09	5 (38%) 0 0	60, 75, 89, 98	0
54	1w	68/76 (89%)	1.72	23 (33%) 0 0	67, 86, 97, 105	0
54	1y	67/76 (88%)	1.22	11 (16%) 1 1	40, 91, 97, 99	0
54	2w	67/76 (88%)	3.49	47 (70%) 0 0	73, 88, 97, 99	0
54	2y	66/76 (86%)	1.16	11 (16%) 1 1	43, 93, 97, 99	0
55	1x	72/77 (93%)	0.36	2 (2%) 53 46	27, 56, 81, 85	0
55	2x	72/77 (93%)	0.64	5 (6%) 16 12	44, 77, 88, 94	0
All	All	20879/21754 (95%)	0.56	1422 (6%) 17 12	16, 61, 86, 106	0

All (1422) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
45	2n	38	GLY	13.6
54	2w	74	C	12.1

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Mol	Chain	Res	Type	RSRZ
22	10	6	GLY	10.8
54	2w	73	A	10.4
22	20	7	LEU	10.3
44	2m	124	PRO	9.8
54	2w	76	A	9.5
45	2n	39	LEU	9.1
44	1m	124	PRO	8.7
45	2n	25	VAL	8.6
44	2m	123	ALA	8.6
22	10	4	LYS	8.4
50	2s	31	ILE	8.4
44	2m	60	VAL	8.1
21	2Z	144	LEU	8.1
38	2g	82	GLY	8.1
54	2w	72	C	8.0
22	10	5	LYS	7.9
22	10	7	LEU	7.7
21	2Z	156	LYS	7.7
54	2w	75	C	7.7
26	24	51	ASP	7.6
44	1m	2	ALA	7.4
38	1g	83	ALA	7.3
44	2m	6	GLY	7.3
38	1g	79	ARG	7.3
22	10	3	HIS	7.2
54	2w	45	U	7.1
54	1w	44	G	7.0
22	20	2	ALA	7.0
21	1Z	1	MET	7.0
54	1w	74	C	6.9
54	2w	71	G	6.9
41	2j	10	GLY	6.7
41	2j	47	PHE	6.6
22	20	4	LYS	6.6
18	2W	112	GLY	6.6
54	2w	44	G	6.5
22	20	5	LYS	6.5
33	2b	165	VAL	6.5
54	2y	36	A	6.5
22	10	2	ALA	6.4
22	20	3	HIS	6.4
54	1w	75	C	6.4

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Mol	Chain	Res	Type	RSRZ
38	1g	82	GLY	6.3
54	1y	35	A	6.2
3	2D	2	ALA	6.2
53	2v	24	A	6.1
54	1w	76	A	6.1
22	20	6	GLY	6.1
35	2d	168	ARG	6.1
38	1g	80	VAL	6.1
50	2s	79	THR	6.0
21	2Z	140	ASP	6.0
54	1w	73	A	6.0
45	2n	50	LYS	6.0
34	2c	158	GLY	6.0
32	2a	1034	G	6.0
50	2s	30	LEU	5.9
54	2w	3	C	5.9
54	2w	31	A	5.8
45	2n	42	ILE	5.8
45	2n	44	LEU	5.8
1	2A	2154	G	5.8
38	1g	84	ASN	5.7
38	1g	85	TYR	5.7
54	2w	70	G	5.7
35	2d	146	ILE	5.7
45	2n	7	ILE	5.7
26	24	49	PHE	5.7
44	2m	90	LEU	5.6
38	2g	80	VAL	5.6
21	2Z	170	THR	5.6
36	2e	12	LEU	5.5
34	2c	12	LEU	5.5
45	2n	36	PHE	5.5
45	2n	51	GLY	5.5
34	2c	60	ALA	5.4
44	2m	5	ALA	5.4
34	2c	33	LEU	5.4
44	2m	66	LEU	5.4
45	2n	37	PHE	5.4
1	1A	885	C	5.4
21	2Z	143	GLY	5.4
41	2j	85	LEU	5.4
1	1A	888	C	5.4

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Mol	Chain	Res	Type	RSRZ
35	2d	183	GLY	5.3
34	2c	182	ILE	5.3
45	2n	34	TYR	5.3
21	2Z	155	LEU	5.3
45	2n	61	TRP	5.3
1	2A	883	G	5.2
50	2s	49	ILE	5.2
33	2b	201	ILE	5.2
44	1m	123	ALA	5.2
1	2A	888	C	5.2
21	2Z	145	GLU	5.2
21	2Z	141	VAL	5.1
34	2c	6	HIS	5.1
45	2n	29	ARG	5.1
50	2s	40	ILE	5.1
21	2Z	50	GLN	5.1
38	2g	83	ALA	5.1
1	1A	896	A	5.0
33	2b	187	LEU	5.0
9	2N	104	LYS	5.0
26	24	50	VAL	5.0
1	1A	1095	A	4.9
53	2v	23	A	4.9
45	2n	53	LEU	4.9
50	2s	41	VAL	4.9
34	2c	8	ILE	4.9
32	2a	1036	G	4.9
12	2Q	33	GLY	4.9
54	2w	69	G	4.9
38	2g	81	GLY	4.9
54	2w	28	G	4.8
21	2Z	154	ASP	4.8
45	2n	10	ALA	4.8
12	2Q	79	LEU	4.8
1	2A	884	C	4.7
32	2a	1030(B)	C	4.7
36	2e	109	ILE	4.7
21	1Z	147	GLY	4.7
34	2c	198	VAL	4.7
1	2A	2146	C	4.7
12	2Q	5	ARG	4.7
27	15	60	VAL	4.7

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Mol	Chain	Res	Type	RSRZ
22	10	8	GLY	4.7
45	2n	55	GLY	4.7
1	1A	2141	G	4.7
40	2i	17	VAL	4.6
45	2n	56	VAL	4.6
41	2j	48	THR	4.6
26	24	57	GLU	4.6
54	2w	56	C	4.6
35	2d	158	ILE	4.6
45	1n	2	ALA	4.6
42	1k	60	ALA	4.6
44	2m	92	HIS	4.6
45	2n	14	PRO	4.6
34	2c	145	GLY	4.6
54	1y	24	G	4.5
12	2Q	6	ARG	4.5
20	2Y	44	ILE	4.5
12	2Q	104	PHE	4.5
35	2d	166	LYS	4.5
6	2G	5	VAL	4.5
54	2w	29	G	4.5
21	2Z	153	SER	4.5
54	1y	36	A	4.5
21	2Z	149	SER	4.5
50	2s	35	SER	4.5
21	1Z	168	GLU	4.5
33	2b	188	ALA	4.5
53	1v	12	A	4.4
25	23	60	GLU	4.4
43	2l	28	LYS	4.4
23	21	2	SER	4.4
29	17	48	LYS	4.4
34	2c	157	ILE	4.4
44	2m	84	ILE	4.4
32	2a	1030(A)	G	4.4
50	2s	53	ASN	4.4
54	1y	20	U	4.4
36	2e	90	VAL	4.3
34	2c	124	ILE	4.3
41	2j	63	PHE	4.3
41	2j	62	HIS	4.3
43	2l	64	TYR	4.3

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Mol	Chain	Res	Type	RSRZ
45	2n	30	ALA	4.3
38	2g	79	ARG	4.3
49	2r	85	LEU	4.3
54	2w	23	A	4.3
50	2s	83	HIS	4.3
32	1a	1028	C	4.3
32	1a	1257	U	4.3
36	2e	133	TYR	4.3
44	1m	87	TYR	4.3
7	2H	115	VAL	4.2
23	1l	2	SER	4.2
54	2y	34	G	4.2
21	2Z	151	HIS	4.2
6	2G	152	LEU	4.2
1	1A	1509	C	4.2
32	1a	1001(A)	G	4.2
54	2w	2	C	4.2
41	2j	11	PHE	4.2
9	2N	116	LEU	4.2
34	2c	189	ALA	4.2
34	1c	193	TYR	4.2
1	2A	885	C	4.2
12	2Q	65	PHE	4.2
35	2d	188	LEU	4.2
41	2j	65	LEU	4.2
34	2c	39	ILE	4.1
50	2s	82	GLY	4.1
1	2A	1026	U	4.1
21	1Z	169	GLU	4.1
41	2j	55	LYS	4.1
12	2Q	109	VAL	4.1
32	2a	1035	A	4.1
34	2c	53	ALA	4.1
46	1o	88	ARG	4.1
54	2w	5	G	4.1
54	2w	24	G	4.1
36	2e	99	GLY	4.1
34	1c	128	PHE	4.1
50	2s	48	THR	4.1
6	2G	140	ILE	4.1
50	2s	62	ILE	4.1
26	24	45	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
54	1w	72	C	4.1
21	2Z	121	HIS	4.1
43	2l	14	GLY	4.1
38	2g	152	ALA	4.1
50	2s	80	TYR	4.1
42	2k	89	ALA	4.1
19	2X	92	LEU	4.0
38	1g	78	ARG	4.0
41	2j	46	ARG	4.0
1	2A	2155	G	4.0
38	1g	153	HIS	4.0
45	2n	13	THR	4.0
6	2G	157	ILE	4.0
21	2Z	122	ARG	4.0
26	24	59	PHE	4.0
34	2c	184	TYR	4.0
38	2g	154	TYR	4.0
34	2c	180	ALA	4.0
34	1c	39	ILE	4.0
33	2b	214	ILE	4.0
1	1A	884	C	4.0
38	1g	81	GLY	4.0
45	2n	12	ARG	4.0
54	2w	30	G	4.0
35	2d	184	LYS	4.0
33	2b	70	PHE	4.0
1	1A	1176	G	4.0
32	2a	1001(A)	G	4.0
36	2e	10	MET	3.9
1	1A	887	A	3.9
1	1A	886	C	3.9
25	23	26	LEU	3.9
42	2k	50	TYR	3.9
12	2Q	59	ARG	3.9
20	2Y	1	MET	3.9
34	1c	87	LEU	3.9
41	2j	96	ILE	3.9
45	2n	31	ARG	3.9
46	1o	82	ILE	3.9
54	2w	19	G	3.9
39	2h	135	CYS	3.9
42	2k	90	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
45	2n	57	ARG	3.9
54	2w	4	C	3.9
44	2m	95	GLY	3.9
54	2w	47	U	3.9
25	23	35	ARG	3.9
45	2n	35	ARG	3.9
6	2G	35	GLU	3.9
21	2Z	125	LEU	3.9
36	2e	31	LEU	3.9
7	2H	106	THR	3.9
40	2i	114	TYR	3.9
43	2l	39	VAL	3.8
32	2a	1033	G	3.8
33	2b	92	TYR	3.8
21	2Z	46	LYS	3.8
1	2A	2153	G	3.8
7	2H	145	ALA	3.8
36	2e	33	VAL	3.8
2	2B	90	A	3.8
44	2m	103	THR	3.8
12	2Q	15	GLY	3.8
14	2S	5	THR	3.8
45	2n	2	ALA	3.8
1	1A	1096	A	3.8
53	1v	24	A	3.8
53	2v	14	A	3.8
36	2e	13	ILE	3.8
44	2m	78	ILE	3.8
48	2q	30	PRO	3.8
1	1A	2159	G	3.8
39	2h	128	GLY	3.8
1	1A	1097	U	3.8
54	2w	21	A	3.8
45	2n	58	LYS	3.8
35	2d	160	GLN	3.8
52	2u	14	TRP	3.8
1	2A	2156	G	3.7
21	2Z	150	LEU	3.7
54	2y	35	A	3.7
39	2h	94	TYR	3.7
50	2s	52	TYR	3.7
39	2h	83	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
1	2A	1509	C	3.7
34	2c	202	ILE	3.7
21	2Z	139	VAL	3.7
21	1Z	104	PHE	3.7
9	2N	23	LEU	3.7
35	2d	176	LEU	3.7
1	2A	887	A	3.7
38	2g	156	TRP	3.7
38	2g	85	TYR	3.7
21	1Z	165	VAL	3.7
22	20	11	ARG	3.7
54	2w	14	A	3.7
6	2G	39	ILE	3.7
53	1v	13	A	3.7
35	2d	64	LEU	3.7
9	2N	47	ALA	3.7
33	2b	37	ASN	3.7
41	2j	98	ILE	3.7
43	2l	94	PRO	3.7
1	2A	2160	G	3.7
34	2c	58	GLU	3.7
44	2m	67	GLU	3.6
12	2Q	10	ARG	3.6
1	1A	883	G	3.6
44	2m	119	GLY	3.6
35	1d	204	ILE	3.6
39	2h	93	VAL	3.6
42	1k	68	ALA	3.6
38	1g	156	TRP	3.6
40	2i	109	VAL	3.6
46	1o	87	ILE	3.6
45	2n	11	LYS	3.6
9	2N	26	LEU	3.6
33	2b	216	SER	3.6
54	2w	6	G	3.6
6	2G	34	LEU	3.6
12	2Q	103	MET	3.6
41	2j	54	PHE	3.6
53	2v	12	A	3.6
50	2s	50	ALA	3.6
33	2b	51	LEU	3.6
3	1D	276	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
12	2Q	114	ALA	3.6
21	2Z	172	ALA	3.6
40	2i	127	LYS	3.6
44	2m	102	ARG	3.6
12	2Q	108	GLY	3.6
43	2l	8	ASN	3.6
43	2l	56	ALA	3.5
1	2A	896	A	3.5
26	24	55	ARG	3.5
35	1d	167	GLY	3.5
34	2c	160	ALA	3.5
43	2l	18	VAL	3.5
22	20	10	THR	3.5
6	2G	133	LEU	3.5
38	2g	7	ALA	3.5
35	2d	112	VAL	3.5
1	2A	2897	U	3.5
33	2b	44	LEU	3.5
49	1r	78	LEU	3.5
35	2d	179	GLU	3.5
1	1A	2158	A	3.5
42	1k	98	LEU	3.5
52	2u	16	GLY	3.5
21	2Z	148	ASP	3.5
33	2b	200	ILE	3.5
36	2e	11	ILE	3.5
35	2d	19	LEU	3.5
42	1k	42	TRP	3.5
44	1m	96	LEU	3.5
1	2A	886	C	3.5
32	1a	1036	G	3.5
54	2w	42	C	3.5
21	2Z	105	VAL	3.5
35	2d	148	VAL	3.5
38	1g	86	GLN	3.5
3	1D	275	LYS	3.4
21	2Z	80	ARG	3.5
46	1o	57	LEU	3.5
50	2s	71	LEU	3.5
32	1a	1030(B)	C	3.4
32	2a	1001	A	3.4
41	2j	50	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
9	2N	102	ALA	3.4
6	2G	29	TRP	3.4
44	2m	121	LYS	3.4
1	1A	2131	G	3.4
54	2w	22	G	3.4
35	2d	20	TYR	3.4
51	2t	24	LEU	3.4
32	2a	1030	C	3.4
50	2s	14	HIS	3.4
1	2A	899	A	3.4
50	2s	66	MET	3.4
12	2Q	32	TYR	3.4
6	2G	2	PRO	3.4
12	2Q	90	VAL	3.4
33	2b	115	LEU	3.4
35	1d	168	ARG	3.4
54	2w	41	C	3.4
6	2G	142	PRO	3.4
7	2H	113	VAL	3.4
20	2Y	45	VAL	3.4
36	2e	98	THR	3.4
45	2n	8	GLU	3.4
44	2m	87	TYR	3.4
10	1O	91	LEU	3.4
7	2H	169	VAL	3.4
48	1q	27	PHE	3.3
20	2Y	5	MET	3.3
26	24	32	TYR	3.3
34	2c	21	ARG	3.3
45	2n	22	THR	3.3
1	2A	2157	G	3.3
6	2G	28	VAL	3.3
39	2h	104	ARG	3.3
42	1k	63	LEU	3.3
12	2Q	132	VAL	3.3
54	1w	70	G	3.3
34	2c	190	ARG	3.3
44	2m	71	ARG	3.3
37	1f	21	LEU	3.3
12	2Q	93	TYR	3.3
21	1Z	100	VAL	3.3
41	2j	6	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
43	2l	95	GLY	3.3
1	2A	2159	G	3.3
12	2Q	37	LEU	3.3
22	20	76	GLY	3.3
33	2b	203	GLY	3.3
54	2w	38	A	3.3
26	24	40	HIS	3.2
7	2H	148	ILE	3.2
26	24	53	GLU	3.2
53	1v	14	A	3.2
39	2h	133	LEU	3.2
1	1A	897	C	3.2
42	2k	25	TYR	3.2
7	2H	105	LEU	3.2
1	1A	2151	G	3.2
1	2A	882	G	3.2
14	2S	20	ARG	3.2
54	1w	71	G	3.2
54	2w	13	C	3.2
54	2w	12	U	3.2
40	2i	115	GLY	3.2
21	1Z	164	ALA	3.2
45	2n	23	ARG	3.2
50	1s	81	ARG	3.2
50	1s	40	ILE	3.2
36	2e	8	GLU	3.2
25	23	28	LEU	3.2
40	2i	79	LEU	3.2
1	2A	897	C	3.2
1	2A	2896	C	3.2
33	2b	66	GLY	3.2
40	2i	80	GLY	3.2
44	2m	68	GLY	3.2
41	2j	44	VAL	3.2
14	2S	32	LEU	3.2
32	2a	1219	U	3.2
34	2c	59	ARG	3.2
35	2d	181	MET	3.2
39	2h	91	ARG	3.2
54	1y	12	U	3.2
33	2b	152	PHE	3.2
40	2i	36	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
12	2Q	86	GLY	3.2
14	2S	58	LEU	3.2
17	2V	71	LEU	3.2
36	2e	43	LEU	3.2
1	2A	229	A	3.1
34	2c	206	GLU	3.1
35	2d	121	VAL	3.1
47	2p	9	PHE	3.1
1	1A	889	C	3.1
1	1A	1064	C	3.1
1	1A	2129	C	3.1
45	2n	26	ARG	3.1
54	2w	15	G	3.1
35	2d	33	MET	3.1
34	2c	37	GLN	3.1
46	1o	89	GLY	3.1
43	2l	32	PHE	3.1
12	2Q	28	ALA	3.1
35	2d	108	LEU	3.1
47	1p	7	ALA	3.1
7	2H	166	GLY	3.1
3	2D	275	LYS	3.1
12	2Q	63	LYS	3.1
49	1r	79	LEU	3.1
42	1k	25	TYR	3.1
50	2s	67	VAL	3.1
45	2n	47	LEU	3.1
26	24	52	THR	3.1
34	2c	13	GLY	3.1
41	1j	10	GLY	3.1
29	17	47	ARG	3.1
36	2e	81	GLU	3.1
36	2e	120	THR	3.1
21	2Z	96	VAL	3.1
25	23	6	VAL	3.1
1	2A	2140	C	3.1
25	23	23	LEU	3.1
42	1k	64	ALA	3.1
33	2b	211	ILE	3.1
46	1o	78	TYR	3.0
36	1e	6	PHE	3.0
1	1A	892	G	3.0

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Mol	Chain	Res	Type	RSRZ
32	2a	1220	G	3.0
35	2d	150	GLU	3.0
44	2m	122	LYS	3.0
54	2w	58	A	3.0
39	2h	65	TYR	3.0
1	2A	2144	U	3.0
32	2a	1257	U	3.0
42	1k	57	THR	3.0
35	2d	105	VAL	3.0
39	2h	2	LEU	3.0
40	2i	76	ALA	3.0
1	1A	2140	C	3.0
1	1A	2146	C	3.0
1	2A	2145	C	3.0
41	2j	60	ARG	3.0
45	2n	46	GLU	3.0
1	1A	2132	U	3.0
45	2n	18	VAL	3.0
50	2s	81	ARG	3.0
12	2Q	40	ALA	3.0
45	1n	7	ILE	3.0
1	2A	2802	G	3.0
45	2n	49	HIS	3.0
33	2b	163	PHE	3.0
34	2c	15	THR	3.0
29	27	46	VAL	3.0
34	2c	91	LEU	3.0
35	1d	11	LEU	3.0
35	1d	78	LEU	3.0
7	2H	89	ILE	3.0
36	2e	9	LYS	3.0
50	2s	57	HIS	3.0
29	27	47	ARG	3.0
54	2w	68	C	3.0
50	2s	15	LEU	3.0
21	2Z	152	ALA	3.0
48	1q	28	PRO	3.0
52	1u	11	GLY	3.0
22	20	45	PHE	3.0
40	2i	33	PHE	3.0
9	2N	13	TRP	3.0
49	1r	40	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
21	2Z	51	ALA	3.0
32	1a	160	A	3.0
9	2N	98	VAL	3.0
41	2j	90	LEU	3.0
22	20	13	GLY	3.0
54	1w	1	G	2.9
54	2y	65	G	2.9
32	1a	344	A	2.9
10	2O	8	LEU	2.9
28	26	28	ARG	2.9
43	2l	15	ARG	2.9
34	2c	200	ALA	2.9
42	2k	35	PRO	2.9
35	2d	70	ILE	2.9
1	1A	2142	C	2.9
17	2V	73	SER	2.9
50	2s	38	SER	2.9
1	1A	1093	G	2.9
21	2Z	157	LEU	2.9
34	2c	85	ARG	2.9
35	2d	159	ARG	2.9
36	2e	29	GLY	2.9
21	1Z	120	ILE	2.9
26	24	18	CYS	2.9
45	2n	24	CYS	2.9
35	2d	110	PHE	2.9
6	1G	152	LEU	2.9
34	2c	193	TYR	2.9
20	2Y	42	VAL	2.9
7	2H	102	ALA	2.9
10	2O	81	ASP	2.9
53	1v	23	A	2.9
39	2h	111	ILE	2.9
44	2m	4	ILE	2.9
34	2c	80	GLY	2.9
40	2i	7	THR	2.9
38	1g	154	TYR	2.9
3	1D	2	ALA	2.9
12	2Q	91	GLU	2.9
21	2Z	138	GLU	2.9
35	2d	98	GLU	2.9
49	1r	73	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
6	2G	115	ARG	2.9
21	2Z	53	ILE	2.9
34	1c	124	ILE	2.9
36	1e	89	ILE	2.9
44	1m	91	ARG	2.9
41	2j	67	THR	2.9
50	2s	33	THR	2.9
10	2O	58	VAL	2.9
12	2Q	106	VAL	2.9
35	2d	177	ASP	2.9
48	2q	100	LYS	2.9
32	1a	345	C	2.9
54	1w	41	C	2.9
1	2A	1042	G	2.9
6	2G	19	LEU	2.9
34	1c	15	THR	2.9
42	1k	47	VAL	2.9
43	2l	55	VAL	2.9
45	2n	59	ALA	2.9
1	1A	1026	U	2.9
35	2d	130	GLY	2.9
43	2l	7	ILE	2.9
48	1q	98	LEU	2.9
6	2G	159	VAL	2.9
9	2N	50	ASP	2.9
36	2e	105	VAL	2.9
38	2g	78	ARG	2.9
21	2Z	25	PRO	2.9
50	2s	24	ALA	2.9
32	1a	161	A	2.8
7	2H	72	ILE	2.8
48	2q	36	ILE	2.8
44	2m	70	LEU	2.8
49	1r	31	LEU	2.8
12	2Q	56	ARG	2.8
48	2q	32	TYR	2.8
1	2A	2602	A	2.8
39	2h	92	ARG	2.8
1	2A	1041	C	2.8
1	2A	2139	C	2.8
12	1Q	81	VAL	2.8
12	2Q	81	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
14	1S	37	ALA	2.8
23	11	62	VAL	2.8
44	1m	122	LYS	2.8
4	2E	71	GLY	2.8
34	2c	18	TRP	2.8
41	2j	68	HIS	2.8
10	2O	19	ILE	2.8
12	2Q	66	ILE	2.8
5	2F	140	LEU	2.8
32	1a	1034	G	2.8
6	2G	182	LYS	2.8
1	2A	2803	C	2.8
9	2N	9	VAL	2.8
35	2d	128	VAL	2.8
44	2m	15	VAL	2.8
44	2m	72	ALA	2.8
54	1w	2	C	2.8
21	1Z	99	TYR	2.8
25	23	11	SER	2.8
52	1u	14	TRP	2.8
12	2Q	64	ILE	2.8
34	2c	17	ASP	2.8
3	2D	38	LYS	2.8
35	2d	169	LYS	2.8
42	1k	81	ASP	2.8
25	23	54	VAL	2.8
40	1i	113	LYS	2.8
50	2s	69	HIS	2.8
20	2Y	55	TYR	2.8
35	2d	122	ARG	2.8
12	2Q	3	MET	2.8
41	2j	12	ASP	2.8
32	1a	1531	A	2.8
36	2e	89	ILE	2.8
54	1w	29	G	2.8
54	2w	18	G	2.8
54	2w	43	C	2.8
44	2m	94	ARG	2.8
35	1d	170	VAL	2.7
23	11	26	ARG	2.7
45	2n	41	ARG	2.7
49	2r	87	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	1A	2602	A	2.7
54	1y	13	C	2.7
7	2H	114	VAL	2.7
26	14	50	VAL	2.7
43	2l	96	VAL	2.7
48	2q	28	PRO	2.7
50	2s	42	PRO	2.7
10	2O	7	TYR	2.7
35	2d	120	LEU	2.7
36	2e	107	ARG	2.7
20	2Y	65	ALA	2.7
35	2d	182	LYS	2.7
42	1k	24	SER	2.7
42	1k	61	ALA	2.7
45	1n	56	VAL	2.7
46	1o	60	VAL	2.7
51	1t	76	ALA	2.7
32	1a	1002	G	2.7
32	2a	1202	G	2.7
21	2Z	99	TYR	2.7
14	2S	35	ILE	2.7
36	2e	135	THR	2.7
42	1k	87	THR	2.7
44	2m	120	LYS	2.7
21	2Z	95	PRO	2.7
9	2N	14	VAL	2.7
12	2Q	102	VAL	2.7
34	2c	207	VAL	2.7
36	2e	104	ALA	2.7
46	2o	60	VAL	2.7
1	2A	2161	C	2.7
12	2Q	61	GLY	2.7
28	26	4	GLU	2.7
54	1y	23	A	2.7
1	2A	1115	G	2.7
55	2x	70	G	2.7
34	2c	134	ILE	2.7
43	2l	31	PRO	2.7
10	2O	57	VAL	2.7
17	2V	72	VAL	2.7
21	2Z	79	ARG	2.7
36	1e	136	MET	2.7

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Mol	Chain	Res	Type	RSRZ
21	1Z	102	LEU	2.7
41	2j	8	LEU	2.7
54	2w	11	C	2.7
22	20	9	SER	2.7
23	21	24	ALA	2.7
34	2c	154	SER	2.7
41	2j	66	ARG	2.7
43	1l	16	GLU	2.7
42	1k	78	GLN	2.7
6	1G	173	LEU	2.7
20	2Y	43	ASN	2.7
35	2d	196	LEU	2.7
36	2e	123	LEU	2.7
45	2n	16	PHE	2.7
19	2X	68	ARG	2.7
21	1Z	170	THR	2.7
52	1u	15	ARG	2.7
52	2u	15	ARG	2.7
9	2N	44	PRO	2.7
21	1Z	51	ALA	2.7
54	2w	7	A	2.7
34	2c	4	LYS	2.7
43	2l	13	LYS	2.7
48	2q	33	GLY	2.7
6	2G	136	ARG	2.7
10	2O	18	LYS	2.7
34	1c	134	ILE	2.7
35	2d	127	THR	2.7
1	1A	1078	U	2.6
41	2j	52	GLY	2.6
39	2h	137	VAL	2.6
38	2g	16	LEU	2.6
32	2a	973	G	2.6
7	2H	25	LYS	2.6
9	2N	69	GLN	2.6
21	2Z	137	ILE	2.6
43	2l	85	ILE	2.6
21	2Z	42	VAL	2.6
42	1k	82	VAL	2.6
34	2c	19	GLU	2.6
43	2l	93	LEU	2.6
11	1P	15	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	2A	2131	G	2.6
35	2d	175	SER	2.6
37	2f	59	TYR	2.6
35	2d	37	PRO	2.6
42	1k	80	VAL	2.6
44	1m	121	LYS	2.6
48	2q	23	VAL	2.6
6	1G	139	LEU	2.6
44	1m	94	ARG	2.6
34	2c	159	GLY	2.6
36	2e	17	ALA	2.6
48	1q	37	LYS	2.6
7	2H	111	HIS	2.6
21	1Z	126	VAL	2.6
35	2d	56	VAL	2.6
44	1m	74	VAL	2.6
10	2O	1	MET	2.6
43	2l	60	LEU	2.6
14	2S	12	PHE	2.6
34	2c	28	GLN	2.6
42	2k	36	ASP	2.6
37	1f	81	ILE	2.6
34	2c	174	PRO	2.6
40	1i	125	TYR	2.6
40	2i	49	PRO	2.6
6	1G	136	ARG	2.6
9	2N	45	ASN	2.6
7	2H	107	VAL	2.6
31	29	25	VAL	2.6
54	2y	63	G	2.6
9	2N	85	ILE	2.6
17	2V	50	PRO	2.6
34	2c	57	ILE	2.6
40	2i	123	PRO	2.6
50	2s	77	THR	2.6
46	1o	69	TYR	2.6
55	2x	65	C	2.6
20	2Y	48	ALA	2.6
35	2d	161	ASN	2.6
9	2N	53	VAL	2.6
43	1l	23	LYS	2.6
9	2N	125	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
12	2Q	112	GLU	2.6
34	1c	203	PHE	2.6
10	2O	42	SER	2.6
1	2A	879	G	2.6
32	2a	1021	G	2.6
38	2g	155	ARG	2.6
55	2x	4	G	2.6
12	1Q	32	TYR	2.6
48	2q	95	TYR	2.6
54	2y	62	C	2.6
40	1i	19	LEU	2.6
45	2n	6	LEU	2.6
33	2b	226	ARG	2.6
6	2G	169	ALA	2.5
35	2d	164	ALA	2.5
42	1k	97	ALA	2.5
43	2l	51	ALA	2.5
44	2m	64	TRP	2.5
13	1R	114	VAL	2.5
34	2c	56	ASP	2.5
36	2e	110	LEU	2.5
49	1r	76	LEU	2.5
36	2e	22	GLY	2.5
50	2s	84	GLY	2.5
7	2H	30	LYS	2.5
43	2l	48	PRO	2.5
50	2s	11	VAL	2.5
3	2D	276	LYS	2.5
31	29	13	LYS	2.5
31	29	33	LYS	2.5
43	2l	47	LYS	2.5
1	1A	2138	C	2.5
1	1A	2161	C	2.5
32	1a	163	C	2.5
6	2G	116	ASP	2.5
28	26	2	ALA	2.5
34	1c	8	ILE	2.5
6	2G	3	LEU	2.5
10	2O	10	VAL	2.5
20	2Y	106	LEU	2.5
33	2b	81	VAL	2.5
38	2g	6	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
41	2j	49	VAL	2.5
42	1k	126	ARG	2.5
50	2s	54	GLY	2.5
32	2a	1222	G	2.5
40	2i	90	PRO	2.5
51	1t	55	ILE	2.5
25	23	29	ARG	2.5
39	2h	90	GLY	2.5
12	2Q	77	LYS	2.5
34	1c	65	ALA	2.5
35	2d	89	THR	2.5
38	2g	149	ARG	2.5
39	2h	124	ALA	2.5
43	2l	29	GLY	2.5
39	2h	112	LEU	2.5
12	2Q	80	GLU	2.5
21	2Z	3	TYR	2.5
35	2d	106	TYR	2.5
32	2a	1196	U	2.5
54	1w	45	U	2.5
3	1D	5	LYS	2.5
9	2N	61	ARG	2.5
40	2i	15	ALA	2.5
48	2q	90	ILE	2.5
21	2Z	76	LEU	2.5
34	2c	89	GLU	2.5
34	2c	101	LEU	2.5
35	1d	62	GLN	2.5
35	1d	64	LEU	2.5
46	1o	62	GLN	2.5
3	1D	205	VAL	2.5
7	2H	24	VAL	2.5
35	2d	104	VAL	2.5
54	1w	24	G	2.5
9	2N	51	PHE	2.5
1	1A	1060	U	2.5
36	2e	24	ARG	2.5
39	2h	84	ARG	2.5
53	1v	25	U	2.5
14	2S	34	HIS	2.5
44	2m	75	ALA	2.5
1	1A	1847	A	2.5

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Mol	Chain	Res	Type	RSRZ
20	2Y	63	LYS	2.5
19	2X	18	TYR	2.5
40	2i	125	TYR	2.5
32	2a	1017	G	2.5
6	2G	134	GLY	2.4
12	2Q	19	GLY	2.4
10	2O	53	LYS	2.4
12	2Q	36	ALA	2.4
29	27	45	ALA	2.4
31	29	15	LYS	2.4
3	2D	271	ILE	2.4
37	1f	48	LEU	2.4
39	1h	6	ILE	2.4
47	1p	19	ILE	2.4
26	24	56	VAL	2.4
35	1d	105	VAL	2.4
39	2h	61	VAL	2.4
47	2p	48	TRP	2.4
54	2w	9	A	2.4
45	2n	40	CYS	2.4
35	2d	69	GLY	2.4
43	2l	100	ILE	2.4
44	1m	90	LEU	2.4
12	1Q	59	ARG	2.4
21	1Z	128	VAL	2.4
31	29	16	VAL	2.4
34	1c	127	ARG	2.4
39	2h	122	ARG	2.4
34	2c	23	TYR	2.4
34	2c	36	ASP	2.4
7	1H	166	GLY	2.4
11	2P	20	GLY	2.4
25	23	27	GLY	2.4
34	1c	155	GLY	2.4
54	1w	31	A	2.4
9	2N	43	THR	2.4
21	2Z	164	ALA	2.4
13	2R	65	LEU	2.4
36	2e	14	ARG	2.4
39	2h	134	ILE	2.4
42	2k	96	ARG	2.4
6	2G	30	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
42	1k	43	SER	2.4
12	2Q	18	LYS	2.4
25	23	9	VAL	2.4
31	29	12	ASP	2.4
21	1Z	167	PRO	2.4
21	2Z	55	HIS	2.4
12	2Q	2	LEU	2.4
12	2Q	110	THR	2.4
21	2Z	173	ALA	2.4
38	2g	147	ALA	2.4
46	1o	68	ARG	2.4
50	2s	75	ALA	2.4
50	2s	78	ARG	2.4
36	2e	131	ILE	2.4
41	2j	61	GLU	2.4
33	2b	197	VAL	2.4
34	2c	66	VAL	2.4
1	2A	1117	G	2.4
6	2G	181	ARG	2.4
38	2g	4	ARG	2.4
41	2j	56	HIS	2.4
43	2l	25	PRO	2.4
6	2G	139	LEU	2.4
16	1U	4	ALA	2.4
34	2c	52	LEU	2.4
35	1d	202	LEU	2.4
35	2d	32	ALA	2.4
45	1n	59	ALA	2.4
32	1a	162	A	2.4
36	1e	118	ILE	2.4
37	1f	55	ASP	2.4
39	2h	131	GLY	2.4
53	2v	21	C	2.4
54	2y	33	U	2.4
55	2x	66	C	2.4
31	29	24	TYR	2.4
40	1i	117	HIS	2.4
7	2H	103	LEU	2.4
16	2U	20	LEU	2.4
34	2c	87	LEU	2.4
34	2c	49	SER	2.4
13	1R	34	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
6	2G	109	VAL	2.4
39	1h	93	VAL	2.4
1	1A	1077	A	2.4
11	1P	102	ARG	2.4
34	1c	126	ARG	2.4
45	1n	17	LYS	2.4
33	2b	34	ALA	2.4
34	2c	94	LEU	2.4
43	2l	62	SER	2.4
1	2A	2793	G	2.4
12	2Q	89	ASN	2.4
34	2c	9	GLY	2.4
14	2S	33	LYS	2.4
36	1e	129	ILE	2.4
54	2w	57	G	2.4
5	1F	72	ARG	2.4
12	2Q	29	PHE	2.4
16	2U	40	PHE	2.4
34	2c	179	ARG	2.4
40	2i	108	VAL	2.4
43	2l	16	GLU	2.4
47	1p	59	TRP	2.4
26	24	63	TYR	2.3
29	27	1	MET	2.3
34	2c	201	TYR	2.3
54	1y	38	A	2.3
12	1Q	43	THR	2.3
12	2Q	31	ASP	2.3
27	25	29	THR	2.3
34	2c	204	LEU	2.3
36	1e	95	ALA	2.3
40	2i	19	LEU	2.3
40	2i	78	LYS	2.3
16	1U	17	ILE	2.3
35	2d	187	ARG	2.3
3	1D	113	VAL	2.3
21	2Z	126	VAL	2.3
33	1b	165	VAL	2.3
36	2e	6	PHE	2.3
42	1k	84	VAL	2.3
43	1l	18	VAL	2.3
1	2A	2112	G	2.3

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Mol	Chain	Res	Type	RSRZ
32	2a	1221	G	2.3
1	2A	614(A)	U	2.3
42	1k	20	TYR	2.3
10	1O	122	LEU	2.3
1	2A	2158	A	2.3
12	2Q	44	ALA	2.3
21	2Z	52	SER	2.3
34	1c	196	LEU	2.3
35	2d	157	LEU	2.3
36	1e	134	ALA	2.3
36	2e	132	ALA	2.3
37	1f	53	ALA	2.3
54	1w	23	A	2.3
54	2w	26	A	2.3
54	2w	67	C	2.3
54	2y	64	A	2.3
25	23	30	ARG	2.3
42	2k	108	ILE	2.3
9	2N	62	VAL	2.3
31	29	11	CYS	2.3
21	2Z	98	MET	2.3
4	1E	195	LEU	2.3
35	2d	162	LEU	2.3
41	1j	60	ARG	2.3
43	2l	10	LEU	2.3
52	2u	13	ILE	2.3
54	1w	42	C	2.3
54	2w	40	C	2.3
8	2I	19	VAL	2.3
16	2U	90	VAL	2.3
36	2e	45	PHE	2.3
34	2c	7	PRO	2.3
4	2E	182	LEU	2.3
33	2b	33	TYR	2.3
35	1d	21	LEU	2.3
40	2i	9	ARG	2.3
44	1m	75	ALA	2.3
35	2d	18	LYS	2.3
42	1k	21	ILE	2.3
5	2F	37	VAL	2.3
9	2N	46	VAL	2.3
10	1O	115	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
38	1g	87	VAL	2.3
21	2Z	93	ASP	2.3
32	1a	1001	A	2.3
28	26	50	ARG	2.3
33	2b	220	ASP	2.3
42	1k	18	ARG	2.3
50	2s	13	ASP	2.3
35	1d	101	LEU	2.3
45	2n	32	SER	2.3
48	2q	74	LEU	2.3
9	2N	57	ALA	2.3
21	1Z	69	THR	2.3
33	2b	161	ALA	2.3
42	1k	75	TYR	2.3
50	2s	32	LYS	2.3
36	2e	80	ILE	2.3
28	26	5	VAL	2.3
6	2G	156	ASP	2.3
54	2y	29	G	2.3
12	2Q	84	GLY	2.3
11	1P	108	LYS	2.3
33	2b	215	LEU	2.3
41	2j	13	HIS	2.3
42	2k	66	LEU	2.3
34	1c	201	TYR	2.3
40	2i	106	ALA	2.3
14	2S	40	ILE	2.3
43	2l	70	ILE	2.3
21	1Z	161	VAL	2.3
45	1n	29	ARG	2.3
47	1p	21	VAL	2.3
50	1s	58	VAL	2.3
9	2N	20	GLY	2.3
19	2X	94	GLY	2.3
34	1c	80	GLY	2.3
43	2l	63	GLY	2.3
1	1A	2149	G	2.3
3	2D	37	LEU	2.3
9	2N	107	LEU	2.3
11	1P	99	LEU	2.3
35	1d	97	LEU	2.3
54	1y	5	G	2.3

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Mol	Chain	Res	Type	RSRZ
1	2A	2174	C	2.3
4	1E	28	ALA	2.3
27	15	2	ALA	2.3
40	2i	82	ALA	2.3
42	1k	89	ALA	2.3
38	1g	151	TYR	2.3
32	1a	1030(D)	A	2.3
12	2Q	87	LYS	2.3
33	2b	58	ILE	2.3
6	2G	160	VAL	2.3
36	2e	82	VAL	2.3
40	2i	28	VAL	2.3
38	1g	73	MET	2.2
39	2h	99	GLU	2.2
36	1e	132	ALA	2.2
42	2k	23	ALA	2.2
3	1D	38	LYS	2.2
6	1G	51	ARG	2.2
35	1d	54	TYR	2.2
40	1i	116	LYS	2.2
40	2i	62	TYR	2.2
54	1w	25	C	2.2
54	2w	27	G	2.2
21	1Z	154	ASP	2.2
21	2Z	124	ILE	2.2
25	23	13	ILE	2.2
32	1a	1503	A	2.2
40	2i	26	VAL	2.2
42	1k	30	VAL	2.2
50	2s	58	VAL	2.2
12	1Q	139	GLU	2.2
21	1Z	101	PRO	2.2
46	1o	56	LEU	2.2
6	1G	182	LYS	2.2
21	2Z	4	ARG	2.2
21	2Z	21	ALA	2.2
48	2q	91	ARG	2.2
33	2b	31	TYR	2.2
1	2A	2794	C	2.2
22	20	8	GLY	2.2
1	1A	2162	G	2.2
31	19	7	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
31	19	17	ILE	2.2
37	1f	58	GLY	2.2
45	2n	52	GLN	2.2
55	1x	67	C	2.2
54	2y	5	G	2.2
43	2l	65	GLU	2.2
39	2h	64	LYS	2.2
48	2q	6	LEU	2.2
1	1A	1081	U	2.2
52	2u	22	ARG	2.2
42	2k	60	ALA	2.2
6	2G	161	THR	2.2
28	16	47	THR	2.2
7	2H	164	TYR	2.2
31	29	37	GLY	2.2
35	2d	185	PHE	2.2
33	2b	222	ILE	2.2
47	1p	2	VAL	2.2
48	2q	59	ILE	2.2
36	2e	130	ASN	2.2
21	2Z	70	LEU	2.2
40	1i	47	LEU	2.2
50	1s	83	HIS	2.2
7	2H	165	ALA	2.2
40	1i	15	ALA	2.2
42	1k	94	ALA	2.2
5	1F	70	THR	2.2
54	1w	14	A	2.2
6	2G	49	ASP	2.2
35	2d	90	GLY	2.2
35	1d	110	PHE	2.2
42	1k	59	TYR	2.2
5	2F	193	VAL	2.2
34	2c	120	VAL	2.2
7	1H	2	SER	2.2
6	1G	106	LEU	2.2
23	11	98	LEU	2.2
33	2b	118	LEU	2.2
45	2n	27	CYS	2.2
49	1r	85	LEU	2.2
31	19	1	MET	2.2
26	24	19	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
32	1a	117	G	2.2
52	2u	17	THR	2.2
54	2w	10	G	2.2
1	1A	2135	A	2.2
19	2X	69	TYR	2.2
21	2Z	48	PHE	2.2
54	1w	21	A	2.2
35	1d	73	ARG	2.2
40	2i	63	ILE	2.2
41	2j	59	SER	2.2
50	2s	28	LYS	2.2
35	2d	23	GLY	2.2
40	2i	27	THR	2.2
52	1u	17	THR	2.2
35	2d	139	ARG	2.2
35	2d	207	TYR	2.2
3	1D	145	VAL	2.2
3	2D	18	VAL	2.2
34	1c	14	ILE	2.2
1	2A	6	A	2.2
12	2Q	85	LYS	2.2
54	1y	21	A	2.2
35	2d	94	LEU	2.2
10	2O	11	ALA	2.2
11	2P	1	MET	2.2
9	2N	93	THR	2.2
31	29	9	ARG	2.2
1	1A	2130	U	2.1
40	1i	126	SER	2.1
42	2k	51	LYS	2.1
28	26	52	VAL	2.1
35	1d	70	ILE	2.1
46	2o	45	VAL	2.1
25	23	53	LEU	2.1
32	2a	1002	G	2.1
1	1A	529	A	2.1
35	1d	50	ARG	2.1
35	2d	47	ARG	2.1
1	1A	1175	U	2.1
4	2E	196	VAL	2.1
7	2H	144	VAL	2.1
21	1Z	124	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
36	2e	129	ILE	2.1
41	2j	72	VAL	2.1
42	2k	93	GLN	2.1
34	1c	34	LEU	2.1
46	1o	31	LEU	2.1
49	2r	66	LEU	2.1
23	2l	28	GLY	2.1
50	2s	68	GLY	2.1
35	1d	209	ARG	2.1
15	2T	46	GLU	2.1
12	2Q	113	GLN	2.1
33	2b	55	PHE	2.1
42	1k	62	GLN	2.1
42	2k	125	PHE	2.1
10	1O	52	VAL	2.1
12	2Q	97	VAL	2.1
15	1T	89	VAL	2.1
41	1j	94	VAL	2.1
42	1k	50	TYR	2.1
11	2P	5	ASP	2.1
21	2Z	163	LEU	2.1
43	1l	60	LEU	2.1
44	2m	88	ARG	2.1
45	2n	19	ARG	2.1
54	2w	25	C	2.1
55	2x	3	C	2.1
35	2d	34	GLU	2.1
35	2d	165	MET	2.1
40	2i	110	GLU	2.1
42	1k	15	ALA	2.1
5	2F	172	TRP	2.1
38	2g	86	GLN	2.1
34	2c	10	PHE	2.1
45	2n	60	SER	2.1
49	1r	29	PHE	2.1
1	1A	2152	G	2.1
1	2A	2133	G	2.1
54	1w	30	G	2.1
54	1y	34	G	2.1
3	2D	216	GLY	2.1
5	2F	208	GLY	2.1
12	1Q	66	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
21	2Z	102	LEU	2.1
31	29	19	ARG	2.1
34	2c	155	GLY	2.1
35	1d	148	VAL	2.1
35	2d	198	VAL	2.1
39	1h	4	ASP	2.1
43	2l	69	TYR	2.1
1	2A	2132	U	2.1
36	2e	16	THR	2.1
6	1G	115	ARG	2.1
6	2G	85	GLY	2.1
12	1Q	5	ARG	2.1
41	2j	89	ASP	2.1
5	2F	82	ILE	2.1
38	1g	141	VAL	2.1
35	1d	138	TYR	2.1
42	1k	29	ILE	2.1
50	1s	60	VAL	2.1
12	2Q	99	PRO	2.1
16	2U	108	GLU	2.1
5	1F	42	ALA	2.1
25	23	51	ALA	2.1
1	1A	2145	C	2.1
39	1h	3	THR	2.1
40	2i	126	SER	2.1
48	2q	27	PHE	2.1
23	2l	22	GLY	2.1
50	2s	12	ASP	2.1
6	2G	43	LEU	2.1
7	2H	35	VAL	2.1
8	1I	38	LEU	2.1
37	1f	98	LEU	2.1
39	2h	132	GLU	2.1
10	2O	47	ILE	2.1
13	1R	97	VAL	2.1
38	1g	105	VAL	2.1
46	1o	34	LEU	2.1
51	2t	13	LEU	2.1
21	2Z	167	PRO	2.1
35	1d	4	TYR	2.1
31	19	34	GLN	2.1
1	2A	2319	G	2.1

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Mol	Chain	Res	Type	RSRZ
29	17	45	ALA	2.1
32	2a	983	A	2.1
42	2k	65	ALA	2.1
54	2y	38	A	2.1
32	1a	1532	U	2.1
34	2c	3	ASN	2.1
35	2d	118	ARG	2.1
48	2q	7	THR	2.1
12	1Q	65	PHE	2.1
35	2d	152	SER	2.1
1	1A	1092	C	2.1
7	2H	159	GLU	2.1
16	1U	26	GLY	2.1
34	2c	2	GLY	2.1
54	1w	13	C	2.1
41	1j	65	LEU	2.1
7	1H	21	PRO	2.1
15	1T	48	ILE	2.1
35	1d	207	TYR	2.1
40	2i	88	TYR	2.1
45	2n	17	LYS	2.1
42	1k	65	ALA	2.1
3	1D	50	THR	2.1
21	1Z	166	SER	2.1
21	2Z	129	SER	2.1
35	1d	137	SER	2.1
42	1k	77	MET	2.1
44	2m	73	GLU	2.1
1	2A	2310	A	2.1
16	1U	43	GLY	2.1
44	2m	112	GLY	2.1
1	2A	2111	C	2.0
12	2Q	17	LEU	2.0
21	1Z	70	LEU	2.0
21	1Z	155	LEU	2.0
35	1d	120	LEU	2.0
35	2d	135	LEU	2.0
39	1h	112	LEU	2.0
43	2l	27	LEU	2.0
47	2p	74	LEU	2.0
35	1d	140	VAL	2.0
3	1D	75	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
21	1Z	133	ILE	2.0
6	2G	146	TYR	2.0
45	2n	45	ARG	2.0
21	2Z	106	GLY	2.0
21	2Z	147	GLY	2.0
34	2c	194	GLY	2.0
35	1d	208	SER	2.0
12	2Q	125	LEU	2.0
47	1p	73	LEU	2.0
49	2r	26	LEU	2.0
55	1x	47	U	2.0
1	2A	2148	G	2.0
2	2B	89	G	2.0
9	2N	11	PRO	2.0
29	17	46	VAL	2.0
34	1c	64	VAL	2.0
34	2c	153	VAL	2.0
44	2m	74	VAL	2.0
47	2p	51	VAL	2.0
50	2s	47	HIS	2.0
53	1v	15	A	2.0
9	2N	97	ARG	2.0
10	2O	86	ILE	2.0
12	2Q	16	ARG	2.0
34	1c	164	ARG	2.0
36	2e	101	ILE	2.0
42	2k	91	ARG	2.0
48	2q	60	ILE	2.0
6	1G	48	GLU	2.0
7	2H	94	TYR	2.0
35	2d	163	GLU	2.0
42	2k	59	TYR	2.0
9	2N	92	ALA	2.0
34	2c	100	ALA	2.0
38	1g	147	ALA	2.0
38	2g	145	ALA	2.0
42	2k	117	ASN	2.0
11	2P	28	GLY	2.0
21	2Z	45	ASP	2.0
23	21	29	GLY	2.0
34	2c	197	GLY	2.0
35	1d	61	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
42	1k	33	THR	2.0
43	1l	61	THR	2.0
44	1m	95	GLY	2.0
3	2D	206	LEU	2.0
41	1j	85	LEU	2.0
7	2H	124	GLU	2.0
12	1Q	78	PRO	2.0
26	24	58	ARG	2.0
39	2h	12	ARG	2.0
44	2m	80	ARG	2.0
50	2s	60	VAL	2.0
6	2G	77	ILE	2.0
39	2h	86	ILE	2.0
1	2A	652(B)	A	2.0
9	2N	109	LYS	2.0
1	1A	388	G	2.0
10	2O	41	ALA	2.0
34	1c	72	LYS	2.0
44	2m	42	ALA	2.0
44	2m	65	LYS	2.0
45	2n	4	LYS	2.0
48	2q	42	TYR	2.0
54	1w	10	G	2.0
50	1s	56	GLN	2.0
33	2b	101	MET	2.0
4	2E	195	LEU	2.0
6	2G	95	ARG	2.0
18	2W	82	LEU	2.0
20	2Y	31	LEU	2.0
35	1d	157	LEU	2.0
37	1f	79	LEU	2.0
43	2l	77	LEU	2.0
51	1t	80	ARG	2.0
21	1Z	39	VAL	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	PSU	2y	55	20/21	0.68	0.23	80,96,106,120	0
54	7MG	2y	46	24/25	0.76	0.17	84,98,104,130	0
54	PSU	1y	55	20/21	0.79	0.29	80,96,105,117	0
54	4SU	2y	8	20/21	0.79	0.15	80,97,107,114	0
54	5MU	2y	54	21/22	0.80	0.27	81,94,101,117	0
54	PSU	2y	32	20/21	0.81	0.33	74,85,99,103	0
54	4SU	2w	8	20/21	0.82	0.28	68,89,101,117	0
54	PSU	2w	55	20/21	0.82	0.35	63,84,92,92	0
54	7MG	2w	46	24/25	0.82	0.41	73,93,103,114	0
54	7MG	1y	46	24/25	0.84	0.22	81,96,103,124	0
54	PSU	1w	55	20/21	0.84	0.28	61,81,88,95	0
54	MIA	2y	37	22/30	0.84	0.34	68,84,93,122	0
54	PSU	2y	39	20/21	0.84	0.30	75,83,94,99	0
54	5MU	1y	54	21/22	0.84	0.21	70,86,99,113	0
54	PSU	1y	32	20/21	0.85	0.36	72,86,96,100	0
54	7MG	1w	46	24/25	0.86	0.20	66,84,103,123	0
54	4SU	1y	8	20/21	0.87	0.18	79,87,95,95	0
54	5MU	2w	54	21/22	0.88	0.25	55,78,91,98	0
32	M2G	2a	966	25/26	0.88	0.22	52,72,85,96	0
54	MIA	2w	37	22/30	0.89	0.26	60,78,83,89	0
54	PSU	2w	32	20/21	0.89	0.35	69,80,91,97	0
55	4SU	2x	8	20/21	0.89	0.15	65,81,88,92	0
55	5MU	2x	54	21/22	0.89	0.23	68,79,84,102	0
43	0TD	2l	92	10/11	0.90	0.20	62,70,72,90	0
54	PSU	1y	39	20/21	0.90	0.27	73,83,89,90	0
54	MIA	1y	37	22/30	0.91	0.27	64,78,83,86	0
54	PSU	1w	32	20/21	0.91	0.24	67,79,90,93	0
32	4OC	2a	1402	22/23	0.91	0.19	48,64,76,83	0
55	PSU	2x	55	20/21	0.91	0.20	63,74,87,92	0
54	PSU	2w	39	20/21	0.92	0.39	68,76,83,83	0
32	2MG	2a	1207	24/25	0.92	0.17	69,80,93,94	0
54	4SU	1w	8	20/21	0.93	0.18	63,75,89,89	0
32	5MC	2a	967	21/22	0.93	0.19	61,67,75,87	0
43	0TD	1l	92	10/11	0.93	0.21	48,55,61,77	0
32	PSU	2a	516	20/21	0.93	0.16	56,70,76,84	0
54	PSU	1w	39	20/21	0.94	0.24	65,73,79,81	0
1	5MU	2A	1915	21/22	0.94	0.14	59,69,77,91	0
32	5MC	2a	1404	21/22	0.94	0.19	50,61,68,76	0
32	PSU	1a	516	20/21	0.94	0.15	58,67,74,78	0
1	PSU	2A	1911	20/21	0.94	0.18	40,58,64,67	0
32	5MC	2a	1400	21/22	0.94	0.23	61,73,83,87	0
1	PSU	1A	1917	20/21	0.95	0.18	44,58,66,67	0
54	5MU	1w	54	21/22	0.95	0.24	48,66,72,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	2MG	1a	1207	24/25	0.95	0.15	49,69,77,81	0
55	4SU	1x	8	20/21	0.95	0.19	41,59,76,88	0
1	PSU	2A	1917	20/21	0.95	0.16	48,61,71,72	0
1	4OC	2A	1920	21/23	0.95	0.20	46,54,60,72	0
55	PSU	1x	55	20/21	0.95	0.18	48,55,72,72	0
54	MIA	1w	37	29/30	0.95	0.26	41,59,74,84	0
32	MA6	2a	1519	24/25	0.96	0.25	48,62,68,73	0
1	5MU	1A	1915	21/22	0.96	0.20	54,67,70,77	0
32	5MC	1a	967	21/22	0.96	0.21	42,52,66,70	0
32	4OC	1a	1402	22/23	0.96	0.21	35,45,57,62	0
32	7MG	1a	527	24/25	0.96	0.17	35,51,55,62	0
32	7MG	2a	527	24/25	0.96	0.19	54,66,75,89	0
55	5MC	2x	32	21/22	0.96	0.19	63,73,82,83	0
55	5MU	1x	54	21/22	0.96	0.18	40,62,68,69	0
32	5MC	2a	1407	21/22	0.96	0.18	38,51,59,70	0
32	UR3	2a	1498	21/22	0.96	0.21	36,56,67,69	0
32	MA6	2a	1518	24/25	0.96	0.20	44,63,70,76	0
1	PSU	2A	2605	20/21	0.97	0.19	20,31,35,36	0
32	5MC	1a	1400	21/22	0.97	0.19	36,52,62,67	0
1	4OC	1A	1920	21/23	0.97	0.24	37,52,60,63	0
1	PSU	1A	1911	20/21	0.97	0.21	41,51,62,64	0
1	5MU	2A	1939	21/22	0.97	0.18	25,32,39,43	0
1	5MC	1A	1942	21/22	0.97	0.19	37,49,54,58	0
32	M2G	1a	966	25/26	0.97	0.20	39,49,58,74	0
55	5MC	1x	32	21/22	0.97	0.23	44,53,60,62	0
1	5MC	2A	1942	21/22	0.97	0.18	41,51,58,67	0
1	5MC	1A	1962	21/22	0.97	0.22	25,36,43,50	0
32	MA6	1a	1519	24/25	0.97	0.24	24,42,50,65	0
1	5MC	2A	1962	21/22	0.97	0.17	27,40,49,52	0
1	2MU	2A	2552	21/23	0.97	0.20	26,32,38,49	0
32	UR3	1a	1498	21/22	0.98	0.22	35,43,51,52	0
1	2MA	2A	2503	23/24	0.98	0.20	21,28,35,40	0
32	MA6	1a	1518	24/25	0.98	0.23	28,42,50,51	0
1	2MU	1A	2552	21/23	0.98	0.21	24,30,37,41	0
1	5MU	1A	1939	21/22	0.98	0.21	24,31,38,39	0
1	PSU	1A	2605	20/21	0.98	0.20	19,24,34,35	0
1	OMG	1A	2251	24/25	0.98	0.22	25,29,37,40	0
32	5MC	1a	1404	21/22	0.98	0.20	30,40,45,48	0
1	OMG	2A	2251	24/25	0.98	0.21	28,33,40,42	0
32	5MC	1a	1407	21/22	0.98	0.22	32,46,51,62	0
1	2MA	1A	2503	23/24	0.98	0.24	18,26,31,35	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1a	1810	1/1	0.42	0.14	90,90,90,90	0
56	MG	1A	3888	1/1	0.44	0.14	89,89,89,89	0
56	MG	1A	3720	1/1	0.59	0.26	71,71,71,71	0
56	MG	2a	1621	1/1	0.60	0.13	74,74,74,74	0
56	MG	2A	3074	1/1	0.61	0.18	54,54,54,54	0
56	MG	2a	1667	1/1	0.61	0.14	73,73,73,73	0
56	MG	2a	1649	1/1	0.62	0.21	71,71,71,71	0
56	MG	1A	3649	1/1	0.62	0.15	58,58,58,58	0
56	MG	2a	1706	1/1	0.63	0.14	75,75,75,75	0
56	MG	1a	1746	1/1	0.64	0.12	85,85,85,85	0
56	MG	1A	3770	1/1	0.65	0.52	63,63,63,63	0
56	MG	1a	1806	1/1	0.65	0.18	68,68,68,68	0
56	MG	1a	1691	1/1	0.67	0.21	66,66,66,66	0
56	MG	2A	3270	1/1	0.68	0.08	38,38,38,38	0
56	MG	2O	8002	1/1	0.68	1.29	112,112,112,112	0
56	MG	1A	3932	1/1	0.68	0.22	56,56,56,56	0
56	MG	1A	3257	1/1	0.69	0.26	65,65,65,65	0
56	MG	2a	1655	1/1	0.69	0.24	64,64,64,64	0
56	MG	2O	102	1/1	0.69	0.23	57,57,57,57	0
56	MG	1A	3183	1/1	0.69	0.21	50,50,50,50	0
59	ZN	24	501	1/1	0.69	0.07	143,143,143,143	0
56	MG	1A	3271	1/1	0.70	0.14	71,71,71,71	0
56	MG	1A	3253	1/1	0.71	0.13	51,51,51,51	0
56	MG	1A	3558	1/1	0.71	0.12	51,51,51,51	0
56	MG	1A	3758	1/1	0.71	0.14	40,40,40,40	0
56	MG	2A	3497	1/1	0.71	0.25	56,56,56,56	0
56	MG	1A	3214	1/1	0.72	0.18	59,59,59,59	0
56	MG	2a	1617	1/1	0.72	0.15	52,52,52,52	0
56	MG	1a	1693	1/1	0.72	0.16	60,60,60,60	0
56	MG	1a	1624	1/1	0.72	0.11	65,65,65,65	0
56	MG	2a	1631	1/1	0.73	0.18	58,58,58,58	0
56	MG	1A	3836	1/1	0.73	0.29	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	1731	1/1	0.73	0.10	65,65,65,65	0
56	MG	1A	3784	1/1	0.73	0.14	63,63,63,63	0
56	MG	1a	1612	1/1	0.74	0.17	63,63,63,63	0
56	MG	1A	3341	1/1	0.74	0.22	60,60,60,60	0
56	MG	1a	1657	1/1	0.74	0.26	56,56,56,56	0
56	MG	2a	1642	1/1	0.74	0.16	66,66,66,66	0
56	MG	1a	1676	1/1	0.74	0.17	64,64,64,64	0
56	MG	1A	3751	1/1	0.74	0.11	63,63,63,63	0
56	MG	2A	3559	1/1	0.74	0.23	59,59,59,59	0
56	MG	2A	3578	1/1	0.74	0.30	65,65,65,65	0
56	MG	2a	1730	1/1	0.74	0.17	71,71,71,71	0
56	MG	1Q	206	1/1	0.74	0.22	54,54,54,54	0
56	MG	10	101	1/1	0.74	0.31	59,59,59,59	0
56	MG	1a	1651	1/1	0.75	0.21	62,62,62,62	0
56	MG	2a	1756	1/1	0.75	0.12	49,49,49,49	0
56	MG	2w	3003	1/1	0.75	0.10	70,70,70,70	0
56	MG	1A	3667	1/1	0.75	0.11	45,45,45,45	0
56	MG	1A	3522	1/1	0.76	0.21	38,38,38,38	0
56	MG	2A	3190	1/1	0.76	0.18	44,44,44,44	0
56	MG	2A	3197	1/1	0.76	0.49	50,50,50,50	0
56	MG	1A	3333	1/1	0.76	0.17	51,51,51,51	0
56	MG	2a	1651	1/1	0.76	0.25	70,70,70,70	0
56	MG	1A	3750	1/1	0.76	0.14	53,53,53,53	0
56	MG	2A	3532	1/1	0.76	0.11	69,69,69,69	0
56	MG	2a	1672	1/1	0.76	0.16	72,72,72,72	0
56	MG	1B	3012	1/1	0.76	0.16	66,66,66,66	0
56	MG	1A	3578	1/1	0.76	0.12	39,39,39,39	0
56	MG	1A	3600	1/1	0.76	0.16	41,41,41,41	0
56	MG	1A	3414	1/1	0.76	0.13	31,31,31,31	0
56	MG	2a	1767	1/1	0.76	0.15	74,74,74,74	0
56	MG	2a	1608	1/1	0.76	0.14	65,65,65,65	0
56	MG	1A	3660	1/1	0.76	0.14	50,50,50,50	0
56	MG	1a	1665	1/1	0.77	0.25	56,56,56,56	0
56	MG	2a	1611	1/1	0.77	0.11	62,62,62,62	0
56	MG	1a	1798	1/1	0.77	0.13	71,71,71,71	0
56	MG	1a	1667	1/1	0.77	0.17	68,68,68,68	0
56	MG	1a	1808	1/1	0.77	0.16	67,67,67,67	0
56	MG	1A	3722	1/1	0.77	0.49	48,48,48,48	0
56	MG	1A	3757	1/1	0.77	0.09	44,44,44,44	0
56	MG	2A	3075	1/1	0.77	0.27	41,41,41,41	0
56	MG	1A	3056	1/1	0.77	0.19	48,48,48,48	0
56	MG	1a	1689	1/1	0.78	0.13	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3266	1/1	0.78	0.17	61,61,61,61	0
56	MG	1A	3847	1/1	0.78	0.52	74,74,74,74	0
56	MG	1a	1717	1/1	0.78	0.31	80,80,80,80	0
56	MG	2A	3201	1/1	0.78	0.23	61,61,61,61	0
56	MG	2A	3222	1/1	0.78	0.17	47,47,47,47	0
56	MG	1A	3376	1/1	0.78	0.15	42,42,42,42	0
56	MG	2A	3285	1/1	0.78	0.12	64,64,64,64	0
56	MG	2A	3396	1/1	0.78	0.16	36,36,36,36	0
56	MG	1a	1761	1/1	0.78	0.30	72,72,72,72	0
56	MG	2A	3514	1/1	0.78	0.17	59,59,59,59	0
56	MG	2A	3530	1/1	0.78	0.10	52,52,52,52	0
56	MG	2a	1724	1/1	0.78	0.16	83,83,83,83	0
56	MG	1A	3210	1/1	0.78	0.12	55,55,55,55	0
56	MG	1A	3605	1/1	0.78	0.09	74,74,74,74	0
56	MG	1A	3783	1/1	0.78	0.15	27,27,27,27	0
56	MG	2B	3001	1/1	0.78	0.27	69,69,69,69	0
56	MG	1A	3182	1/1	0.78	0.24	65,65,65,65	0
56	MG	1a	1826	1/1	0.78	0.20	72,72,72,72	0
56	MG	1A	3597	1/1	0.79	0.18	50,50,50,50	0
56	MG	2A	3328	1/1	0.79	0.12	39,39,39,39	0
56	MG	2a	1625	1/1	0.79	0.15	71,71,71,71	0
56	MG	2a	1629	1/1	0.79	0.19	55,55,55,55	0
56	MG	1A	3662	1/1	0.79	0.20	55,55,55,55	0
56	MG	2A	3492	1/1	0.79	0.14	50,50,50,50	0
56	MG	1A	3872	1/1	0.79	0.11	50,50,50,50	0
56	MG	1a	1831	1/1	0.79	0.11	58,58,58,58	0
56	MG	2A	3025	1/1	0.79	0.20	61,61,61,61	0
56	MG	1A	3515	1/1	0.79	0.17	37,37,37,37	0
56	MG	1a	1697	1/1	0.79	0.14	63,63,63,63	0
56	MG	1a	1644	1/1	0.79	0.23	56,56,56,56	0
56	MG	2A	3603	1/1	0.79	0.18	65,65,65,65	0
56	MG	1A	3893	1/1	0.79	0.08	47,47,47,47	0
56	MG	2F	301	1/1	0.79	0.23	37,37,37,37	0
56	MG	1A	3715	1/1	0.79	0.12	50,50,50,50	0
56	MG	1A	3755	1/1	0.79	0.13	55,55,55,55	0
56	MG	2A	3234	1/1	0.79	0.11	54,54,54,54	0
56	MG	1F	306	1/1	0.79	0.18	46,46,46,46	0
56	MG	1A	3592	1/1	0.80	0.18	32,32,32,32	0
56	MG	1b	3002	1/1	0.80	0.22	74,74,74,74	0
56	MG	2A	3535	1/1	0.80	0.07	62,62,62,62	0
56	MG	2A	3551	1/1	0.80	0.17	51,51,51,51	0
56	MG	1a	1707	1/1	0.80	0.20	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3280	1/1	0.80	0.20	50,50,50,50	0
56	MG	2A	3592	1/1	0.80	0.14	57,57,57,57	0
56	MG	1A	3169	1/1	0.80	0.15	44,44,44,44	0
56	MG	2A	3116	1/1	0.80	0.19	56,56,56,56	0
56	MG	2a	1674	1/1	0.80	0.13	58,58,58,58	0
56	MG	2B	3009	1/1	0.80	0.19	62,62,62,62	0
56	MG	2A	3386	1/1	0.80	0.11	50,50,50,50	0
56	MG	2A	3173	1/1	0.80	0.14	45,45,45,45	0
56	MG	2A	3407	1/1	0.80	0.11	44,44,44,44	0
56	MG	2A	3441	1/1	0.80	0.17	33,33,33,33	0
56	MG	2A	3176	1/1	0.80	0.24	52,52,52,52	0
56	MG	2t	3001	1/1	0.80	0.19	48,48,48,48	0
56	MG	1A	3243	1/1	0.80	0.12	56,56,56,56	0
56	MG	1a	1827	1/1	0.80	0.13	55,55,55,55	0
56	MG	2A	3082	1/1	0.81	0.25	45,45,45,45	0
56	MG	1A	3608	1/1	0.81	0.15	40,40,40,40	0
56	MG	2a	1613	1/1	0.81	0.18	58,58,58,58	0
56	MG	1A	3803	1/1	0.81	0.15	60,60,60,60	0
56	MG	1A	3635	1/1	0.81	0.09	49,49,49,49	0
56	MG	2A	3182	1/1	0.81	0.10	53,53,53,53	0
56	MG	1A	3084	1/1	0.81	0.23	42,42,42,42	0
56	MG	1A	3242	1/1	0.81	0.19	47,47,47,47	0
56	MG	2a	1633	1/1	0.81	0.55	61,61,61,61	0
56	MG	1A	3116	1/1	0.81	0.28	47,47,47,47	0
56	MG	2A	3208	1/1	0.81	0.14	45,45,45,45	0
56	MG	1A	3025	1/1	0.81	0.12	44,44,44,44	0
56	MG	2A	3570	1/1	0.81	0.15	57,57,57,57	0
56	MG	2a	1661	1/1	0.81	0.28	65,65,65,65	0
56	MG	2A	3577	1/1	0.81	0.23	61,61,61,61	0
56	MG	2a	1671	1/1	0.81	0.15	54,54,54,54	0
56	MG	1a	1656	1/1	0.81	0.28	46,46,46,46	0
56	MG	1x	3005	1/1	0.81	0.20	66,66,66,66	0
56	MG	1A	3285	1/1	0.81	0.18	49,49,49,49	0
56	MG	2A	3636	1/1	0.81	0.17	55,55,55,55	0
56	MG	2A	3643	1/1	0.81	0.15	38,38,38,38	0
56	MG	2A	3651	1/1	0.81	0.14	55,55,55,55	0
56	MG	2a	1740	1/1	0.81	0.14	82,82,82,82	0
56	MG	2A	3051	1/1	0.81	0.15	61,61,61,61	0
56	MG	2A	3385	1/1	0.81	0.13	43,43,43,43	0
56	MG	1A	3292	1/1	0.81	0.14	49,49,49,49	0
56	MG	1a	1773	1/1	0.81	0.10	64,64,64,64	0
56	MG	2A	3402	1/1	0.81	0.14	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3298	1/1	0.82	0.12	39,39,39,39	0
56	MG	1A	3367	1/1	0.82	0.20	55,55,55,55	0
56	MG	2A	3347	1/1	0.82	0.15	45,45,45,45	0
56	MG	2A	3368	1/1	0.82	0.14	38,38,38,38	0
56	MG	1A	3023	1/1	0.82	0.36	57,57,57,57	0
56	MG	2A	3617	1/1	0.82	0.09	54,54,54,54	0
56	MG	2A	3632	1/1	0.82	0.21	58,58,58,58	0
56	MG	1A	3773	1/1	0.82	0.25	41,41,41,41	0
56	MG	1A	3960	1/1	0.82	0.16	38,38,38,38	0
56	MG	1B	3005	1/1	0.82	0.18	58,58,58,58	0
56	MG	1A	3225	1/1	0.82	0.23	55,55,55,55	0
56	MG	1B	3014	1/1	0.82	0.22	63,63,63,63	0
56	MG	2a	1680	1/1	0.82	0.15	73,73,73,73	0
56	MG	2A	3491	1/1	0.82	0.16	49,49,49,49	0
56	MG	2F	304	1/1	0.82	0.14	54,54,54,54	0
56	MG	2a	1729	1/1	0.82	0.12	65,65,65,65	0
56	MG	1a	1815	1/1	0.82	0.08	76,76,76,76	0
56	MG	1A	3236	1/1	0.82	0.17	52,52,52,52	0
56	MG	1Q	205	1/1	0.82	0.24	58,58,58,58	0
56	MG	1A	3074	1/1	0.82	0.18	45,45,45,45	0
56	MG	1A	3015	1/1	0.82	0.20	43,43,43,43	0
56	MG	2a	1779	1/1	0.82	0.16	74,74,74,74	0
56	MG	2a	1791	1/1	0.82	0.13	63,63,63,63	0
56	MG	1A	3098	1/1	0.82	0.17	56,56,56,56	0
56	MG	1A	3099	1/1	0.82	0.17	51,51,51,51	0
56	MG	1a	1721	1/1	0.82	0.17	66,66,66,66	0
56	MG	1a	1828	1/1	0.83	0.12	62,62,62,62	0
56	MG	1a	1681	1/1	0.83	0.27	54,54,54,54	0
56	MG	2A	3179	1/1	0.83	0.12	45,45,45,45	0
56	MG	1A	3880	1/1	0.83	0.12	37,37,37,37	0
56	MG	1A	3670	1/1	0.83	0.23	58,58,58,58	0
56	MG	2A	3024	1/1	0.83	0.16	33,33,33,33	0
56	MG	1A	3761	1/1	0.83	0.13	56,56,56,56	0
56	MG	1A	3213	1/1	0.83	0.24	42,42,42,42	0
56	MG	1A	3057	1/1	0.83	0.12	44,44,44,44	0
56	MG	2A	3233	1/1	0.83	0.22	44,44,44,44	0
56	MG	2a	1736	1/1	0.83	0.10	68,68,68,68	0
56	MG	1A	3264	1/1	0.83	0.15	64,64,64,64	0
56	MG	2A	3248	1/1	0.83	0.12	52,52,52,52	0
56	MG	19	101	1/1	0.83	0.20	41,41,41,41	0
56	MG	2a	1769	1/1	0.83	0.11	73,73,73,73	0
56	MG	2a	1774	1/1	0.83	0.17	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2a	1777	1/1	0.83	0.18	77,77,77,77	0
56	MG	2a	1647	1/1	0.83	0.13	64,64,64,64	0
56	MG	2A	3667	1/1	0.83	0.14	53,53,53,53	0
56	MG	2A	3520	1/1	0.83	0.11	51,51,51,51	0
56	MG	2A	3102	1/1	0.83	0.15	49,49,49,49	0
56	MG	1B	3010	1/1	0.83	0.11	68,68,68,68	0
56	MG	2A	3011	1/1	0.84	0.18	41,41,41,41	0
56	MG	1B	3007	1/1	0.84	0.20	53,53,53,53	0
56	MG	1B	3008	1/1	0.84	0.17	57,57,57,57	0
56	MG	1A	3494	1/1	0.84	0.10	47,47,47,47	0
56	MG	2A	3061	1/1	0.84	0.15	43,43,43,43	0
56	MG	2A	3425	1/1	0.84	0.16	38,38,38,38	0
56	MG	2A	3064	1/1	0.84	0.15	58,58,58,58	0
56	MG	2A	3474	1/1	0.84	0.10	44,44,44,44	0
56	MG	1A	3207	1/1	0.84	0.12	52,52,52,52	0
56	MG	1A	3788	1/1	0.84	0.16	24,24,24,24	0
56	MG	2A	3493	1/1	0.84	0.12	62,62,62,62	0
56	MG	1F	303	1/1	0.84	0.18	34,34,34,34	0
56	MG	2A	3501	1/1	0.84	0.07	46,46,46,46	0
56	MG	2A	3512	1/1	0.84	0.12	52,52,52,52	0
56	MG	2A	3086	1/1	0.84	0.13	43,43,43,43	0
56	MG	1A	3738	1/1	0.84	0.39	44,44,44,44	0
56	MG	2a	1664	1/1	0.84	0.14	71,71,71,71	0
56	MG	1N	3006	1/1	0.84	0.63	50,50,50,50	0
56	MG	1A	3085	1/1	0.84	0.18	51,51,51,51	0
56	MG	1a	1743	1/1	0.84	0.25	63,63,63,63	0
56	MG	1A	3075	1/1	0.84	0.25	43,43,43,43	0
56	MG	1a	1756	1/1	0.84	0.06	65,65,65,65	0
56	MG	1Z	3001	1/1	0.84	0.24	50,50,50,50	0
56	MG	1A	3868	1/1	0.84	0.09	48,48,48,48	0
56	MG	1A	3121	1/1	0.84	0.31	55,55,55,55	0
56	MG	1A	3308	1/1	0.84	0.21	58,58,58,58	0
56	MG	1a	1616	1/1	0.84	0.19	62,62,62,62	0
56	MG	1A	3441	1/1	0.84	0.15	48,48,48,48	0
56	MG	1A	3892	1/1	0.84	0.15	41,41,41,41	0
56	MG	2A	3237	1/1	0.84	0.18	57,57,57,57	0
56	MG	1a	1645	1/1	0.84	0.14	56,56,56,56	0
56	MG	1A	3486	1/1	0.84	0.17	46,46,46,46	0
56	MG	1A	3903	1/1	0.84	0.23	51,51,51,51	0
56	MG	1A	3602	1/1	0.84	0.18	22,22,22,22	0
56	MG	1A	3718	1/1	0.84	0.16	69,69,69,69	0
56	MG	1x	3001	1/1	0.84	0.13	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	2r	101	1/1	0.84	0.14	66,66,66,66	0
56	MG	1A	3778	1/1	0.84	0.10	48,48,48,48	0
56	MG	2A	3371	1/1	0.84	0.10	49,49,49,49	0
56	MG	20	101	1/1	0.84	0.12	57,57,57,57	0
61	FME	2x	103	10/11	0.84	0.39	36,58,64,90	10
56	MG	1w	3003	1/1	0.85	0.32	78,78,78,78	0
56	MG	1A	3742	1/1	0.85	0.22	37,37,37,37	0
56	MG	2A	3227	1/1	0.85	0.16	48,48,48,48	0
56	MG	1A	3943	1/1	0.85	0.17	42,42,42,42	0
56	MG	1A	3747	1/1	0.85	0.18	49,49,49,49	0
56	MG	1A	3267	1/1	0.85	0.15	53,53,53,53	0
56	MG	2A	3244	1/1	0.85	0.14	43,43,43,43	0
56	MG	2a	1648	1/1	0.85	0.12	61,61,61,61	0
56	MG	2A	3538	1/1	0.85	0.10	53,53,53,53	0
56	MG	1A	3610	1/1	0.85	0.08	56,56,56,56	0
56	MG	1A	3677	1/1	0.85	0.13	57,57,57,57	0
56	MG	2a	1657	1/1	0.85	0.14	54,54,54,54	0
56	MG	1A	3239	1/1	0.85	0.13	56,56,56,56	0
56	MG	2A	3575	1/1	0.85	0.08	57,57,57,57	0
56	MG	1A	3639	1/1	0.85	0.16	39,39,39,39	0
56	MG	1A	3363	1/1	0.85	0.15	58,58,58,58	0
56	MG	2A	3585	1/1	0.85	0.27	44,44,44,44	0
56	MG	2A	3345	1/1	0.85	0.15	40,40,40,40	0
56	MG	1E	302	1/1	0.85	0.26	43,43,43,43	0
56	MG	2A	3357	1/1	0.85	0.16	49,49,49,49	0
56	MG	2a	1709	1/1	0.85	0.12	68,68,68,68	0
56	MG	1A	3473	1/1	0.85	0.18	26,26,26,26	0
56	MG	1a	1664	1/1	0.85	0.10	57,57,57,57	0
56	MG	2A	3376	1/1	0.85	0.12	41,41,41,41	0
56	MG	2A	3087	1/1	0.85	0.16	55,55,55,55	0
56	MG	1A	3732	1/1	0.85	0.09	60,60,60,60	0
56	MG	1A	3777	1/1	0.85	0.10	42,42,42,42	0
56	MG	2A	3169	1/1	0.85	0.14	41,41,41,41	0
56	MG	2D	301	1/1	0.85	0.49	39,39,39,39	0
56	MG	2A	3172	1/1	0.85	0.11	59,59,59,59	0
56	MG	2a	1771	1/1	0.85	0.23	63,63,63,63	0
56	MG	2A	3414	1/1	0.85	0.15	40,40,40,40	0
56	MG	1a	1672	1/1	0.85	0.11	55,55,55,55	0
56	MG	2Q	204	1/1	0.85	0.29	44,44,44,44	0
56	MG	1O	205	1/1	0.85	0.15	55,55,55,55	0
56	MG	1A	3244	1/1	0.85	0.34	39,39,39,39	0
56	MG	1A	3779	1/1	0.85	0.34	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	1R	203	1/1	0.85	0.19	44,44,44,44	0
56	MG	1a	1692	1/1	0.85	0.17	60,60,60,60	0
56	MG	1d	503	1/1	0.85	0.08	66,66,66,66	0
56	MG	28	101	1/1	0.86	0.20	57,57,57,57	0
56	MG	2A	3424	1/1	0.86	0.22	43,43,43,43	0
56	MG	1A	3401	1/1	0.86	0.16	38,38,38,38	0
56	MG	1a	1613	1/1	0.86	0.20	62,62,62,62	0
56	MG	1A	3931	1/1	0.86	0.19	57,57,57,57	0
56	MG	1A	3409	1/1	0.86	0.08	34,34,34,34	0
56	MG	2a	1622	1/1	0.86	0.13	44,44,44,44	0
56	MG	1a	1630	1/1	0.86	0.19	57,57,57,57	0
56	MG	1a	1634	1/1	0.86	0.17	61,61,61,61	0
56	MG	2A	3187	1/1	0.86	0.14	60,60,60,60	0
56	MG	1A	3165	1/1	0.86	0.15	38,38,38,38	0
56	MG	2a	1634	1/1	0.86	0.15	53,53,53,53	0
56	MG	1A	3434	1/1	0.86	0.10	39,39,39,39	0
56	MG	1A	3347	1/1	0.86	0.27	54,54,54,54	0
56	MG	1A	3460	1/1	0.86	0.15	37,37,37,37	0
56	MG	2A	3521	1/1	0.86	0.16	63,63,63,63	0
56	MG	2A	3522	1/1	0.86	0.13	53,53,53,53	0
56	MG	2A	3212	1/1	0.86	0.18	55,55,55,55	0
56	MG	2A	3217	1/1	0.86	0.23	60,60,60,60	0
56	MG	1A	3462	1/1	0.86	0.14	53,53,53,53	0
56	MG	1A	3734	1/1	0.86	0.17	48,48,48,48	0
56	MG	1A	3799	1/1	0.86	0.36	55,55,55,55	0
56	MG	1A	3360	1/1	0.86	0.21	50,50,50,50	0
56	MG	1B	3021	1/1	0.86	0.10	48,48,48,48	0
56	MG	1B	3025	1/1	0.86	0.14	49,49,49,49	0
56	MG	1A	3095	1/1	0.86	0.22	54,54,54,54	0
56	MG	2a	1695	1/1	0.86	0.18	54,54,54,54	0
56	MG	2a	1696	1/1	0.86	0.20	50,50,50,50	0
56	MG	1A	3220	1/1	0.86	0.36	48,48,48,48	0
56	MG	2A	3281	1/1	0.86	0.14	40,40,40,40	0
56	MG	1A	3851	1/1	0.86	0.23	45,45,45,45	0
56	MG	2A	3297	1/1	0.86	0.15	32,32,32,32	0
56	MG	1A	3642	1/1	0.86	0.12	39,39,39,39	0
56	MG	2A	3056	1/1	0.86	0.12	54,54,54,54	0
56	MG	2A	3058	1/1	0.86	0.12	47,47,47,47	0
56	MG	1O	203	1/1	0.86	0.11	52,52,52,52	0
56	MG	1A	3644	1/1	0.86	0.07	57,57,57,57	0
56	MG	1A	3874	1/1	0.86	0.19	63,63,63,63	0
56	MG	1A	3498	1/1	0.86	0.14	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	2B	3003	1/1	0.86	0.17	48,48,48,48	0
56	MG	2A	3373	1/1	0.86	0.15	27,27,27,27	0
56	MG	1A	3129	1/1	0.86	0.22	38,38,38,38	0
56	MG	1a	1742	1/1	0.86	0.16	68,68,68,68	0
56	MG	2a	1783	1/1	0.86	0.18	60,60,60,60	0
56	MG	2F	303	1/1	0.86	0.19	58,58,58,58	0
56	MG	2I	202	1/1	0.86	0.19	62,62,62,62	0
56	MG	1A	3380	1/1	0.86	0.20	30,30,30,30	0
56	MG	1A	3385	1/1	0.86	0.18	42,42,42,42	0
56	MG	1A	3898	1/1	0.86	0.20	25,25,25,25	0
57	K	2A	3207	1/1	0.86	0.26	75,75,75,75	0
56	MG	2A	3126	1/1	0.86	0.21	53,53,53,53	0
56	MG	2A	3162	1/1	0.86	0.10	45,45,45,45	0
56	MG	2E	301	1/1	0.87	0.11	36,36,36,36	0
56	MG	1w	3002	1/1	0.87	0.09	56,56,56,56	0
56	MG	1A	3230	1/1	0.87	0.17	39,39,39,39	0
56	MG	2A	3300	1/1	0.87	0.13	29,29,29,29	0
56	MG	1w	3004	1/1	0.87	0.15	51,51,51,51	0
56	MG	2P	201	1/1	0.87	0.12	47,47,47,47	0
56	MG	1A	3135	1/1	0.87	0.14	49,49,49,49	0
56	MG	1A	3555	1/1	0.87	0.12	55,55,55,55	0
56	MG	1A	3275	1/1	0.87	0.14	39,39,39,39	0
56	MG	1a	1661	1/1	0.87	0.13	56,56,56,56	0
56	MG	1A	3564	1/1	0.87	0.26	24,24,24,24	0
56	MG	2A	3026	1/1	0.87	0.09	35,35,35,35	0
56	MG	1A	3717	1/1	0.87	0.19	60,60,60,60	0
56	MG	2A	3382	1/1	0.87	0.10	48,48,48,48	0
56	MG	2A	3052	1/1	0.87	0.19	50,50,50,50	0
56	MG	1A	3276	1/1	0.87	0.24	51,51,51,51	0
56	MG	1a	1669	1/1	0.87	0.26	58,58,58,58	0
56	MG	2A	3399	1/1	0.87	0.16	47,47,47,47	0
56	MG	1A	3018	1/1	0.87	0.21	52,52,52,52	0
56	MG	1A	3117	1/1	0.87	0.26	38,38,38,38	0
56	MG	2A	3066	1/1	0.87	0.14	46,46,46,46	0
56	MG	1A	3800	1/1	0.87	0.19	54,54,54,54	0
56	MG	1a	1686	1/1	0.87	0.16	47,47,47,47	0
56	MG	1A	3726	1/1	0.87	0.15	62,62,62,62	0
56	MG	1A	3805	1/1	0.87	0.19	64,64,64,64	0
56	MG	1A	3806	1/1	0.87	0.12	73,73,73,73	0
56	MG	2A	3100	1/1	0.87	0.10	52,52,52,52	0
56	MG	1A	3811	1/1	0.87	0.12	64,64,64,64	0
56	MG	2a	1659	1/1	0.87	0.32	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3819	1/1	0.87	0.10	51,51,51,51	0
56	MG	2A	3498	1/1	0.87	0.11	37,37,37,37	0
56	MG	1a	1701	1/1	0.87	0.11	52,52,52,52	0
56	MG	2A	3127	1/1	0.87	0.12	50,50,50,50	0
56	MG	1a	1705	1/1	0.87	0.13	56,56,56,56	0
56	MG	1A	3823	1/1	0.87	0.12	67,67,67,67	0
56	MG	1a	1711	1/1	0.87	0.11	49,49,49,49	0
56	MG	1A	3287	1/1	0.87	0.17	47,47,47,47	0
56	MG	1A	3417	1/1	0.87	0.17	32,32,32,32	0
56	MG	1A	3290	1/1	0.87	0.19	33,33,33,33	0
56	MG	2A	3533	1/1	0.87	0.16	26,26,26,26	0
56	MG	1A	3866	1/1	0.87	0.13	44,44,44,44	0
56	MG	1A	3170	1/1	0.87	0.20	39,39,39,39	0
56	MG	1A	3049	1/1	0.87	0.14	60,60,60,60	0
56	MG	1A	3221	1/1	0.87	0.16	48,48,48,48	0
56	MG	17	102	1/1	0.87	0.11	50,50,50,50	0
56	MG	1A	3222	1/1	0.87	0.25	37,37,37,37	0
56	MG	2A	3210	1/1	0.87	0.14	40,40,40,40	0
56	MG	1a	1607	1/1	0.87	0.21	68,68,68,68	0
56	MG	1a	1611	1/1	0.87	0.16	57,57,57,57	0
56	MG	1A	3259	1/1	0.87	0.16	61,61,61,61	0
56	MG	1A	3490	1/1	0.87	0.10	53,53,53,53	0
56	MG	2A	3230	1/1	0.87	0.22	57,57,57,57	0
56	MG	1A	3053	1/1	0.87	0.23	52,52,52,52	0
56	MG	1A	3226	1/1	0.87	0.37	35,35,35,35	0
56	MG	2a	1789	1/1	0.87	0.17	58,58,58,58	0
56	MG	1A	3764	1/1	0.87	0.10	40,40,40,40	0
56	MG	1a	1829	1/1	0.87	0.19	57,57,57,57	0
56	MG	2A	3655	1/1	0.87	0.10	31,31,31,31	0
56	MG	1A	3904	1/1	0.87	0.13	55,55,55,55	0
56	MG	1a	1641	1/1	0.87	0.16	50,50,50,50	0
56	MG	2x	102	1/1	0.87	0.11	58,58,58,58	0
56	MG	2A	3271	1/1	0.87	0.14	34,34,34,34	0
56	MG	1A	3912	1/1	0.87	0.15	35,35,35,35	0
56	MG	1l	203	1/1	0.87	0.17	58,58,58,58	0
56	MG	2E	302	1/1	0.88	0.12	39,39,39,39	0
56	MG	1A	3705	1/1	0.88	0.10	52,52,52,52	0
56	MG	2A	3330	1/1	0.88	0.14	44,44,44,44	0
56	MG	1R	201	1/1	0.88	0.14	34,34,34,34	0
56	MG	2G	3001	1/1	0.88	0.14	54,54,54,54	0
56	MG	1A	3706	1/1	0.88	0.13	51,51,51,51	0
56	MG	1V	201	1/1	0.88	0.15	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	1A	3895	1/1	0.88	0.19	40,40,40,40	0
56	MG	1Z	3003	1/1	0.88	0.18	61,61,61,61	0
56	MG	2A	3065	1/1	0.88	0.19	43,43,43,43	0
56	MG	1Z	3005	1/1	0.88	0.26	56,56,56,56	0
56	MG	2A	3073	1/1	0.88	0.14	46,46,46,46	0
56	MG	1A	3237	1/1	0.88	0.16	44,44,44,44	0
56	MG	13	102	1/1	0.88	0.16	52,52,52,52	0
56	MG	1A	3900	1/1	0.88	0.24	28,28,28,28	0
56	MG	1a	1726	1/1	0.88	0.06	57,57,57,57	0
56	MG	1A	3076	1/1	0.88	0.14	43,43,43,43	0
56	MG	2a	1623	1/1	0.88	0.15	65,65,65,65	0
56	MG	1A	3421	1/1	0.88	0.08	60,60,60,60	0
56	MG	1a	1608	1/1	0.88	0.33	57,57,57,57	0
56	MG	2A	3115	1/1	0.88	0.15	38,38,38,38	0
56	MG	1A	3618	1/1	0.88	0.07	70,70,70,70	0
56	MG	2A	3434	1/1	0.88	0.15	39,39,39,39	0
56	MG	2A	3125	1/1	0.88	0.12	56,56,56,56	0
56	MG	1A	3914	1/1	0.88	0.23	38,38,38,38	0
56	MG	1A	3624	1/1	0.88	0.16	57,57,57,57	0
56	MG	2A	3150	1/1	0.88	0.22	35,35,35,35	0
56	MG	1a	1789	1/1	0.88	0.16	45,45,45,45	0
56	MG	2a	1652	1/1	0.88	0.14	62,62,62,62	0
56	MG	2A	3166	1/1	0.88	0.17	43,43,43,43	0
56	MG	1A	3293	1/1	0.88	0.17	26,26,26,26	0
56	MG	1a	1800	1/1	0.88	0.13	50,50,50,50	0
56	MG	2A	3504	1/1	0.88	0.17	45,45,45,45	0
56	MG	1a	1620	1/1	0.88	0.13	50,50,50,50	0
56	MG	1a	1807	1/1	0.88	0.15	84,84,84,84	0
56	MG	2a	1670	1/1	0.88	0.19	53,53,53,53	0
56	MG	1A	3938	1/1	0.88	0.35	43,43,43,43	0
56	MG	1a	1809	1/1	0.88	0.10	83,83,83,83	0
56	MG	1a	1629	1/1	0.88	0.13	58,58,58,58	0
56	MG	1A	3528	1/1	0.88	0.10	64,64,64,64	0
56	MG	1a	1820	1/1	0.88	0.15	62,62,62,62	0
56	MG	1A	3370	1/1	0.88	0.21	42,42,42,42	0
56	MG	2a	1704	1/1	0.88	0.13	40,40,40,40	0
56	MG	1A	3228	1/1	0.88	0.17	39,39,39,39	0
56	MG	1A	3648	1/1	0.88	0.10	46,46,46,46	0
56	MG	2A	3550	1/1	0.88	0.18	52,52,52,52	0
56	MG	2a	1725	1/1	0.88	0.07	69,69,69,69	0
56	MG	1A	3017	1/1	0.88	0.23	31,31,31,31	0
56	MG	2A	3556	1/1	0.88	0.07	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	2A	3214	1/1	0.88	0.23	41,41,41,41	0
56	MG	2a	1734	1/1	0.88	0.13	70,70,70,70	0
56	MG	2A	3561	1/1	0.88	0.05	71,71,71,71	0
56	MG	2A	3216	1/1	0.88	0.10	43,43,43,43	0
56	MG	1A	3021	1/1	0.88	0.20	50,50,50,50	0
56	MG	1a	1835	1/1	0.88	0.15	57,57,57,57	0
56	MG	1a	1837	1/1	0.88	0.41	60,60,60,60	0
56	MG	1A	3827	1/1	0.88	0.26	51,51,51,51	0
56	MG	1A	3474	1/1	0.88	0.20	29,29,29,29	0
56	MG	1A	3663	1/1	0.88	0.14	46,46,46,46	0
56	MG	1A	3848	1/1	0.88	0.19	29,29,29,29	0
56	MG	1E	301	1/1	0.88	0.19	27,27,27,27	0
56	MG	1A	3483	1/1	0.88	0.17	29,29,29,29	0
56	MG	2A	3250	1/1	0.88	0.12	43,43,43,43	0
56	MG	2j	8002	1/1	0.88	0.10	66,66,66,66	0
56	MG	1A	3248	1/1	0.88	0.10	32,32,32,32	0
56	MG	1A	3674	1/1	0.88	0.12	53,53,53,53	0
56	MG	1A	3356	1/1	0.88	0.13	35,35,35,35	0
56	MG	2w	3001	1/1	0.88	0.20	67,67,67,67	0
56	MG	1A	3766	1/1	0.88	0.10	57,57,57,57	0
56	MG	1A	3699	1/1	0.88	0.16	66,66,66,66	0
56	MG	1A	3701	1/1	0.88	0.14	47,47,47,47	0
56	MG	2A	3043	1/1	0.88	0.26	39,39,39,39	0
56	MG	2A	3323	1/1	0.88	0.09	47,47,47,47	0
56	MG	2A	3615	1/1	0.89	0.13	46,46,46,46	0
56	MG	2A	3616	1/1	0.89	0.17	55,55,55,55	0
56	MG	1a	1836	1/1	0.89	0.17	60,60,60,60	0
56	MG	2A	3622	1/1	0.89	0.26	41,41,41,41	0
56	MG	2A	3224	1/1	0.89	0.10	46,46,46,46	0
56	MG	1A	3196	1/1	0.89	0.15	52,52,52,52	0
56	MG	1A	3083	1/1	0.89	0.24	27,27,27,27	0
56	MG	2A	3644	1/1	0.89	0.40	42,42,42,42	0
56	MG	1A	3850	1/1	0.89	0.25	60,60,60,60	0
56	MG	2A	3653	1/1	0.89	0.20	36,36,36,36	0
56	MG	1F	305	1/1	0.89	0.16	46,46,46,46	0
56	MG	1A	3254	1/1	0.89	0.26	58,58,58,58	0
56	MG	2A	3243	1/1	0.89	0.22	53,53,53,53	0
56	MG	2B	3002	1/1	0.89	0.17	55,55,55,55	0
56	MG	1A	3529	1/1	0.89	0.21	54,54,54,54	0
56	MG	2B	3006	1/1	0.89	0.14	51,51,51,51	0
56	MG	2B	3008	1/1	0.89	0.12	55,55,55,55	0
56	MG	1a	1673	1/1	0.89	0.09	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2B	3014	1/1	0.89	0.26	65,65,65,65	0
56	MG	1A	3429	1/1	0.89	0.23	53,53,53,53	0
56	MG	2A	3252	1/1	0.89	0.09	58,58,58,58	0
56	MG	1O	204	1/1	0.89	0.14	52,52,52,52	0
56	MG	1x	3008	1/1	0.89	0.22	61,61,61,61	0
56	MG	2A	3005	1/1	0.89	0.19	50,50,50,50	0
56	MG	1a	1684	1/1	0.89	0.14	54,54,54,54	0
56	MG	2A	3012	1/1	0.89	0.12	40,40,40,40	0
56	MG	1A	3279	1/1	0.89	0.11	52,52,52,52	0
56	MG	1A	3157	1/1	0.89	0.18	39,39,39,39	0
56	MG	2A	3305	1/1	0.89	0.17	37,37,37,37	0
56	MG	2A	3320	1/1	0.89	0.13	42,42,42,42	0
56	MG	1A	3224	1/1	0.89	0.17	51,51,51,51	0
56	MG	2A	3039	1/1	0.89	0.17	46,46,46,46	0
56	MG	2A	3041	1/1	0.89	0.10	59,59,59,59	0
56	MG	2A	3343	1/1	0.89	0.10	33,33,33,33	0
56	MG	1A	3584	1/1	0.89	0.17	19,19,19,19	0
56	MG	1A	3891	1/1	0.89	0.26	76,76,76,76	0
56	MG	1a	1696	1/1	0.89	0.15	66,66,66,66	0
56	MG	2A	3366	1/1	0.89	0.11	41,41,41,41	0
56	MG	2A	3053	1/1	0.89	0.18	44,44,44,44	0
56	MG	2a	1624	1/1	0.89	0.26	54,54,54,54	0
56	MG	2A	3055	1/1	0.89	0.18	54,54,54,54	0
56	MG	2a	1626	1/1	0.89	0.24	50,50,50,50	0
56	MG	1A	3461	1/1	0.89	0.16	27,27,27,27	0
56	MG	1A	3686	1/1	0.89	0.11	29,29,29,29	0
56	MG	1a	1702	1/1	0.89	0.26	60,60,60,60	0
56	MG	1a	1704	1/1	0.89	0.22	73,73,73,73	0
56	MG	1A	3594	1/1	0.89	0.13	35,35,35,35	0
56	MG	2A	3388	1/1	0.89	0.11	52,52,52,52	0
56	MG	2A	3391	1/1	0.89	0.16	53,53,53,53	0
56	MG	1A	3260	1/1	0.89	0.15	40,40,40,40	0
56	MG	1A	3465	1/1	0.89	0.12	32,32,32,32	0
56	MG	1A	3262	1/1	0.89	0.23	48,48,48,48	0
56	MG	1A	3709	1/1	0.89	0.16	43,43,43,43	0
56	MG	1A	3374	1/1	0.89	0.13	47,47,47,47	0
56	MG	1A	3790	1/1	0.89	0.15	49,49,49,49	0
56	MG	1A	3793	1/1	0.89	0.17	28,28,28,28	0
56	MG	1a	1744	1/1	0.89	0.09	53,53,53,53	0
56	MG	1A	3796	1/1	0.89	0.16	47,47,47,47	0
56	MG	2A	3110	1/1	0.89	0.34	46,46,46,46	0
56	MG	1a	1750	1/1	0.89	0.11	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	1a	1752	1/1	0.89	0.18	59,59,59,59	0
56	MG	1a	1755	1/1	0.89	0.13	57,57,57,57	0
56	MG	1A	3164	1/1	0.89	0.14	51,51,51,51	0
56	MG	1a	1758	1/1	0.89	0.14	55,55,55,55	0
56	MG	2A	3137	1/1	0.89	0.34	42,42,42,42	0
56	MG	1A	3081	1/1	0.89	0.20	43,43,43,43	0
56	MG	2A	3509	1/1	0.89	0.21	50,50,50,50	0
56	MG	1A	3613	1/1	0.89	0.15	36,36,36,36	0
56	MG	2A	3513	1/1	0.89	0.07	50,50,50,50	0
56	MG	2A	3164	1/1	0.89	0.15	47,47,47,47	0
56	MG	1a	1617	1/1	0.89	0.17	47,47,47,47	0
56	MG	1a	1618	1/1	0.89	0.13	64,64,64,64	0
56	MG	1B	3002	1/1	0.89	0.19	48,48,48,48	0
56	MG	2A	3527	1/1	0.89	0.08	53,53,53,53	0
56	MG	2A	3529	1/1	0.89	0.22	57,57,57,57	0
56	MG	2a	1739	1/1	0.89	0.15	74,74,74,74	0
56	MG	1a	1801	1/1	0.89	0.15	54,54,54,54	0
56	MG	2a	1753	1/1	0.89	0.07	80,80,80,80	0
56	MG	1A	3217	1/1	0.89	0.10	42,42,42,42	0
56	MG	1A	3316	1/1	0.89	0.11	44,44,44,44	0
56	MG	1A	3729	1/1	0.89	0.20	39,39,39,39	0
56	MG	1A	3322	1/1	0.89	0.34	55,55,55,55	0
56	MG	2A	3188	1/1	0.89	0.18	50,50,50,50	0
56	MG	1a	1635	1/1	0.89	0.31	50,50,50,50	0
56	MG	2A	3191	1/1	0.89	0.23	58,58,58,58	0
56	MG	2a	1781	1/1	0.89	0.17	66,66,66,66	0
56	MG	1B	3011	1/1	0.89	0.33	54,54,54,54	0
56	MG	2A	3198	1/1	0.89	0.13	42,42,42,42	0
56	MG	2A	3564	1/1	0.89	0.17	45,45,45,45	0
56	MG	2f	3002	1/1	0.89	0.21	61,61,61,61	0
56	MG	2A	3567	1/1	0.89	0.23	58,58,58,58	0
56	MG	1A	3637	1/1	0.89	0.20	39,39,39,39	0
56	MG	1A	3826	1/1	0.89	0.20	37,37,37,37	0
56	MG	2A	3576	1/1	0.89	0.09	59,59,59,59	0
56	MG	1a	1649	1/1	0.89	0.19	56,56,56,56	0
56	MG	1A	3505	1/1	0.89	0.15	28,28,28,28	0
56	MG	1a	1654	1/1	0.89	0.09	54,54,54,54	0
56	MG	1B	3024	1/1	0.89	0.27	63,63,63,63	0
56	MG	1A	3512	1/1	0.89	0.20	53,53,53,53	0
56	MG	2A	3604	1/1	0.89	0.12	45,45,45,45	0
56	MG	2A	3029	1/1	0.90	0.17	47,47,47,47	0
56	MG	1A	3273	1/1	0.90	0.20	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	3775	1/1	0.90	0.12	47,47,47,47	0
56	MG	1A	3440	1/1	0.90	0.16	72,72,72,72	0
56	MG	2A	3296	1/1	0.90	0.18	47,47,47,47	0
56	MG	2A	3046	1/1	0.90	0.12	38,38,38,38	0
56	MG	1A	3080	1/1	0.90	0.24	31,31,31,31	0
56	MG	1A	3178	1/1	0.90	0.27	36,36,36,36	0
56	MG	1a	1603	1/1	0.90	0.21	66,66,66,66	0
56	MG	1a	1604	1/1	0.90	0.11	47,47,47,47	0
56	MG	1a	1734	1/1	0.90	0.16	30,30,30,30	0
56	MG	1A	3697	1/1	0.90	0.12	57,57,57,57	0
56	MG	1A	3910	1/1	0.90	0.30	40,40,40,40	0
56	MG	1a	1609	1/1	0.90	0.12	54,54,54,54	0
56	MG	1A	3070	1/1	0.90	0.11	33,33,33,33	0
56	MG	1a	1748	1/1	0.90	0.10	58,58,58,58	0
56	MG	2E	303	1/1	0.90	0.13	42,42,42,42	0
56	MG	2A	3068	1/1	0.90	0.12	39,39,39,39	0
56	MG	2A	3363	1/1	0.90	0.14	30,30,30,30	0
56	MG	1A	3143	1/1	0.90	0.11	30,30,30,30	0
56	MG	1A	3192	1/1	0.90	0.29	39,39,39,39	0
56	MG	1A	3150	1/1	0.90	0.29	41,41,41,41	0
56	MG	2A	3077	1/1	0.90	0.12	43,43,43,43	0
56	MG	1A	3794	1/1	0.90	0.10	21,21,21,21	0
56	MG	2U	204	1/1	0.90	0.46	45,45,45,45	0
56	MG	2V	201	1/1	0.90	0.11	44,44,44,44	0
56	MG	2A	3084	1/1	0.90	0.10	40,40,40,40	0
56	MG	1A	3199	1/1	0.90	0.30	35,35,35,35	0
56	MG	1a	1759	1/1	0.90	0.13	57,57,57,57	0
56	MG	2a	1603	1/1	0.90	0.20	65,65,65,65	0
56	MG	2A	3096	1/1	0.90	0.17	56,56,56,56	0
56	MG	1A	3948	1/1	0.90	0.18	34,34,34,34	0
56	MG	2A	3393	1/1	0.90	0.09	21,21,21,21	0
56	MG	2a	1616	1/1	0.90	0.20	52,52,52,52	0
56	MG	1A	3475	1/1	0.90	0.15	37,37,37,37	0
56	MG	2A	3398	1/1	0.90	0.04	47,47,47,47	0
56	MG	1a	1776	1/1	0.90	0.14	63,63,63,63	0
56	MG	2A	3112	1/1	0.90	0.31	49,49,49,49	0
56	MG	2A	3404	1/1	0.90	0.14	37,37,37,37	0
56	MG	2A	3113	1/1	0.90	0.22	51,51,51,51	0
56	MG	1A	3964	1/1	0.90	0.18	26,26,26,26	0
56	MG	2a	1628	1/1	0.90	0.13	65,65,65,65	0
56	MG	2A	3416	1/1	0.90	0.20	44,44,44,44	0
56	MG	1a	1794	1/1	0.90	0.17	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1a	1796	1/1	0.90	0.13	40,40,40,40	0
56	MG	1A	3200	1/1	0.90	0.13	49,49,49,49	0
56	MG	2A	3438	1/1	0.90	0.15	44,44,44,44	0
56	MG	2a	1643	1/1	0.90	0.18	58,58,58,58	0
56	MG	1a	1799	1/1	0.90	0.33	85,85,85,85	0
56	MG	2A	3448	1/1	0.90	0.13	47,47,47,47	0
56	MG	2A	3131	1/1	0.90	0.22	49,49,49,49	0
56	MG	2A	3482	1/1	0.90	0.29	46,46,46,46	0
56	MG	2A	3483	1/1	0.90	0.07	61,61,61,61	0
56	MG	1A	3113	1/1	0.90	0.20	40,40,40,40	0
56	MG	2A	3140	1/1	0.90	0.14	50,50,50,50	0
56	MG	1B	3006	1/1	0.90	0.23	44,44,44,44	0
56	MG	2A	3155	1/1	0.90	0.21	43,43,43,43	0
56	MG	1a	1636	1/1	0.90	0.11	53,53,53,53	0
56	MG	1A	3384	1/1	0.90	0.19	52,52,52,52	0
56	MG	2a	1668	1/1	0.90	0.12	64,64,64,64	0
56	MG	1A	3296	1/1	0.90	0.26	40,40,40,40	0
56	MG	1A	3088	1/1	0.90	0.24	54,54,54,54	0
56	MG	1A	3626	1/1	0.90	0.12	56,56,56,56	0
56	MG	2a	1673	1/1	0.90	0.26	60,60,60,60	0
56	MG	1A	3630	1/1	0.90	0.19	35,35,35,35	0
56	MG	2a	1678	1/1	0.90	0.12	64,64,64,64	0
56	MG	1a	1819	1/1	0.90	0.13	61,61,61,61	0
56	MG	1A	3503	1/1	0.90	0.18	33,33,33,33	0
56	MG	1A	3212	1/1	0.90	0.10	67,67,67,67	0
56	MG	1A	3093	1/1	0.90	0.14	43,43,43,43	0
56	MG	2A	3524	1/1	0.90	0.09	56,56,56,56	0
56	MG	1A	3844	1/1	0.90	0.16	64,64,64,64	0
56	MG	2a	1720	1/1	0.90	0.10	53,53,53,53	0
56	MG	1A	3641	1/1	0.90	0.26	35,35,35,35	0
56	MG	1A	3327	1/1	0.90	0.17	44,44,44,44	0
56	MG	1A	3419	1/1	0.90	0.15	43,43,43,43	0
56	MG	1a	1668	1/1	0.90	0.12	52,52,52,52	0
56	MG	2A	3200	1/1	0.90	0.10	46,46,46,46	0
56	MG	1A	3525	1/1	0.90	0.09	53,53,53,53	0
56	MG	2A	3547	1/1	0.90	0.17	37,37,37,37	0
56	MG	2a	1738	1/1	0.90	0.61	76,76,76,76	0
56	MG	1A	3852	1/1	0.90	0.15	38,38,38,38	0
56	MG	1A	3063	1/1	0.90	0.22	36,36,36,36	0
56	MG	2a	1748	1/1	0.90	0.12	77,77,77,77	0
56	MG	1A	3426	1/1	0.90	0.16	51,51,51,51	0
56	MG	2A	3558	1/1	0.90	0.13	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	3760	1/1	0.90	0.12	57,57,57,57	0
56	MG	1A	3532	1/1	0.90	0.17	59,59,59,59	0
56	MG	1a	1685	1/1	0.90	0.07	66,66,66,66	0
56	MG	1O	206	1/1	0.90	0.12	62,62,62,62	0
56	MG	2a	1775	1/1	0.90	0.10	71,71,71,71	0
56	MG	2A	3223	1/1	0.90	0.18	51,51,51,51	0
56	MG	1x	3003	1/1	0.90	0.13	53,53,53,53	0
56	MG	2A	3226	1/1	0.90	0.32	42,42,42,42	0
56	MG	1P	204	1/1	0.90	0.27	42,42,42,42	0
56	MG	1A	3875	1/1	0.90	0.16	32,32,32,32	0
56	MG	2A	3584	1/1	0.90	0.27	58,58,58,58	0
56	MG	1x	3009	1/1	0.90	0.12	58,58,58,58	0
56	MG	2A	3002	1/1	0.90	0.23	53,53,53,53	0
56	MG	1A	3879	1/1	0.90	0.21	54,54,54,54	0
56	MG	2q	3001	1/1	0.90	0.05	66,66,66,66	0
56	MG	2A	3241	1/1	0.90	0.08	42,42,42,42	0
56	MG	2A	3610	1/1	0.90	0.20	32,32,32,32	0
56	MG	1A	3762	1/1	0.90	0.27	31,31,31,31	0
56	MG	1A	3886	1/1	0.90	0.15	50,50,50,50	0
56	MG	2A	3245	1/1	0.90	0.15	42,42,42,42	0
56	MG	1A	3548	1/1	0.90	0.22	47,47,47,47	0
56	MG	1A	3665	1/1	0.90	0.09	53,53,53,53	0
56	MG	1A	3334	1/1	0.90	0.23	54,54,54,54	0
56	MG	2A	3341	1/1	0.91	0.19	45,45,45,45	0
56	MG	2A	3661	1/1	0.91	0.11	41,41,41,41	0
56	MG	1a	1768	1/1	0.91	0.13	56,56,56,56	0
56	MG	1A	3838	1/1	0.91	0.18	38,38,38,38	0
56	MG	1a	1774	1/1	0.91	0.09	48,48,48,48	0
56	MG	2A	3094	1/1	0.91	0.15	43,43,43,43	0
56	MG	2A	3361	1/1	0.91	0.07	58,58,58,58	0
56	MG	1A	3060	1/1	0.91	0.18	31,31,31,31	0
56	MG	1A	3345	1/1	0.91	0.20	35,35,35,35	0
56	MG	1A	3062	1/1	0.91	0.18	50,50,50,50	0
56	MG	1a	1795	1/1	0.91	0.07	64,64,64,64	0
56	MG	2D	303	1/1	0.91	0.63	45,45,45,45	0
56	MG	1A	3349	1/1	0.91	0.30	38,38,38,38	0
56	MG	1a	1642	1/1	0.91	0.18	42,42,42,42	0
56	MG	1A	3352	1/1	0.91	0.20	58,58,58,58	0
56	MG	1D	301	1/1	0.91	0.22	46,46,46,46	0
56	MG	2A	3117	1/1	0.91	0.14	43,43,43,43	0
56	MG	1A	3238	1/1	0.91	0.22	28,28,28,28	0
56	MG	1a	1802	1/1	0.91	0.10	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	2O	8001	1/1	0.91	0.12	52,52,52,52	0
56	MG	1a	1650	1/1	0.91	0.21	55,55,55,55	0
56	MG	2A	3394	1/1	0.91	0.15	45,45,45,45	0
56	MG	2A	3128	1/1	0.91	0.12	49,49,49,49	0
56	MG	1A	3861	1/1	0.91	0.11	26,26,26,26	0
56	MG	1F	302	1/1	0.91	0.10	54,54,54,54	0
56	MG	1A	3452	1/1	0.91	0.15	43,43,43,43	0
56	MG	2A	3141	1/1	0.91	0.12	29,29,29,29	0
56	MG	2O	103	1/1	0.91	0.08	49,49,49,49	0
56	MG	1A	3044	1/1	0.91	0.13	23,23,23,23	0
56	MG	2A	3413	1/1	0.91	0.10	50,50,50,50	0
56	MG	1A	3870	1/1	0.91	0.12	44,44,44,44	0
56	MG	1F	307	1/1	0.91	0.38	57,57,57,57	0
56	MG	1I	3001	1/1	0.91	0.09	58,58,58,58	0
56	MG	2a	1614	1/1	0.91	0.15	71,71,71,71	0
56	MG	1A	3124	1/1	0.91	0.17	51,51,51,51	0
56	MG	1A	3765	1/1	0.91	0.30	46,46,46,46	0
56	MG	2a	1618	1/1	0.91	0.26	67,67,67,67	0
56	MG	1A	3566	1/1	0.91	0.16	55,55,55,55	0
56	MG	1A	3054	1/1	0.91	0.21	54,54,54,54	0
56	MG	1A	3369	1/1	0.91	0.14	40,40,40,40	0
56	MG	2A	3469	1/1	0.91	0.09	46,46,46,46	0
56	MG	2A	3177	1/1	0.91	0.11	37,37,37,37	0
56	MG	2A	3478	1/1	0.91	0.15	56,56,56,56	0
56	MG	1A	3774	1/1	0.91	0.17	42,42,42,42	0
56	MG	1a	1677	1/1	0.91	0.12	56,56,56,56	0
56	MG	2A	3184	1/1	0.91	0.17	46,46,46,46	0
56	MG	1Q	201	1/1	0.91	0.23	30,30,30,30	0
56	MG	1a	1682	1/1	0.91	0.22	57,57,57,57	0
56	MG	2A	3495	1/1	0.91	0.23	61,61,61,61	0
56	MG	1A	3269	1/1	0.91	0.16	30,30,30,30	0
56	MG	1A	3593	1/1	0.91	0.14	29,29,29,29	0
56	MG	2A	3499	1/1	0.91	0.09	52,52,52,52	0
56	MG	1A	3372	1/1	0.91	0.17	52,52,52,52	0
56	MG	1A	3696	1/1	0.91	0.28	38,38,38,38	0
56	MG	1A	3301	1/1	0.91	0.43	38,38,38,38	0
56	MG	2a	1653	1/1	0.91	0.13	51,51,51,51	0
56	MG	1W	3001	1/1	0.91	0.24	43,43,43,43	0
56	MG	1A	3598	1/1	0.91	0.18	42,42,42,42	0
56	MG	2a	1658	1/1	0.91	0.09	69,69,69,69	0
56	MG	1Z	3002	1/1	0.91	0.24	56,56,56,56	0
56	MG	1A	3481	1/1	0.91	0.17	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1Z	3004	1/1	0.91	0.17	52,52,52,52	0
56	MG	2A	3215	1/1	0.91	0.24	50,50,50,50	0
56	MG	2A	3523	1/1	0.91	0.14	54,54,54,54	0
56	MG	1A	3601	1/1	0.91	0.24	45,45,45,45	0
56	MG	1A	3303	1/1	0.91	0.15	34,34,34,34	0
56	MG	1A	3131	1/1	0.91	0.16	44,44,44,44	0
56	MG	1a	1706	1/1	0.91	0.17	66,66,66,66	0
56	MG	1A	3133	1/1	0.91	0.20	44,44,44,44	0
56	MG	2A	3225	1/1	0.91	0.22	53,53,53,53	0
56	MG	1a	1710	1/1	0.91	0.16	61,61,61,61	0
56	MG	2a	1689	1/1	0.91	0.11	61,61,61,61	0
56	MG	2a	1693	1/1	0.91	0.23	47,47,47,47	0
56	MG	1A	3609	1/1	0.91	0.06	43,43,43,43	0
56	MG	2A	3540	1/1	0.91	0.17	43,43,43,43	0
56	MG	2A	3542	1/1	0.91	0.22	37,37,37,37	0
56	MG	2A	3028	1/1	0.91	0.10	43,43,43,43	0
56	MG	2A	3548	1/1	0.91	0.10	35,35,35,35	0
56	MG	2a	1718	1/1	0.91	0.09	51,51,51,51	0
56	MG	2A	3231	1/1	0.91	0.14	49,49,49,49	0
56	MG	2a	1721	1/1	0.91	0.13	61,61,61,61	0
56	MG	2a	1722	1/1	0.91	0.21	57,57,57,57	0
56	MG	1A	3317	1/1	0.91	0.58	39,39,39,39	0
56	MG	2A	3037	1/1	0.91	0.13	42,42,42,42	0
56	MG	2A	3236	1/1	0.91	0.16	55,55,55,55	0
56	MG	1a	1718	1/1	0.91	0.16	54,54,54,54	0
56	MG	2A	3238	1/1	0.91	0.10	42,42,42,42	0
56	MG	1A	3612	1/1	0.91	0.14	30,30,30,30	0
56	MG	2A	3566	1/1	0.91	0.11	38,38,38,38	0
56	MG	1a	1725	1/1	0.91	0.15	54,54,54,54	0
56	MG	1a	1606	1/1	0.91	0.18	54,54,54,54	0
56	MG	2A	3574	1/1	0.91	0.14	43,43,43,43	0
56	MG	1a	1727	1/1	0.91	0.07	65,65,65,65	0
56	MG	1a	1733	1/1	0.91	0.11	33,33,33,33	0
56	MG	2A	3249	1/1	0.91	0.17	30,30,30,30	0
56	MG	2a	1760	1/1	0.91	0.10	54,54,54,54	0
56	MG	1A	3020	1/1	0.91	0.11	23,23,23,23	0
56	MG	1A	3502	1/1	0.91	0.18	23,23,23,23	0
56	MG	1A	3945	1/1	0.91	0.24	39,39,39,39	0
56	MG	2a	1773	1/1	0.91	0.13	66,66,66,66	0
56	MG	1A	3051	1/1	0.91	0.15	38,38,38,38	0
56	MG	2A	3593	1/1	0.91	0.28	56,56,56,56	0
56	MG	2A	3598	1/1	0.91	0.20	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	3815	1/1	0.91	0.14	60,60,60,60	0
56	MG	1A	3817	1/1	0.91	0.11	45,45,45,45	0
56	MG	1A	3278	1/1	0.91	0.18	60,60,60,60	0
56	MG	1A	3507	1/1	0.91	0.19	34,34,34,34	0
56	MG	2a	1790	1/1	0.91	0.19	66,66,66,66	0
56	MG	1a	1753	1/1	0.91	0.12	58,58,58,58	0
56	MG	1A	3631	1/1	0.91	0.10	67,67,67,67	0
56	MG	2A	3619	1/1	0.91	0.12	55,55,55,55	0
56	MG	1A	3235	1/1	0.91	0.47	32,32,32,32	0
56	MG	2A	3309	1/1	0.91	0.19	31,31,31,31	0
56	MG	1a	1621	1/1	0.91	0.14	49,49,49,49	0
56	MG	2A	3640	1/1	0.91	0.11	45,45,45,45	0
56	MG	2A	3641	1/1	0.91	0.11	46,46,46,46	0
56	MG	2w	3002	1/1	0.91	0.11	63,63,63,63	0
56	MG	1A	3830	1/1	0.91	0.14	53,53,53,53	0
56	MG	1A	3337	1/1	0.91	0.15	39,39,39,39	0
56	MG	2A	3645	1/1	0.91	0.14	41,41,41,41	0
56	MG	2A	3083	1/1	0.91	0.14	48,48,48,48	0
56	MG	2A	3333	1/1	0.91	0.20	35,35,35,35	0
56	MG	2A	3291	1/1	0.92	0.17	49,49,49,49	0
56	MG	2A	3639	1/1	0.92	0.11	52,52,52,52	0
56	MG	1A	3282	1/1	0.92	0.13	53,53,53,53	0
56	MG	1G	203	1/1	0.92	0.17	71,71,71,71	0
56	MG	1A	3348	1/1	0.92	0.23	54,54,54,54	0
56	MG	1a	1695	1/1	0.92	0.09	55,55,55,55	0
56	MG	2A	3302	1/1	0.92	0.20	38,38,38,38	0
56	MG	1A	3589	1/1	0.92	0.17	29,29,29,29	0
56	MG	2A	3308	1/1	0.92	0.08	45,45,45,45	0
56	MG	1A	3842	1/1	0.92	0.15	39,39,39,39	0
56	MG	2A	3315	1/1	0.92	0.18	40,40,40,40	0
56	MG	1A	3187	1/1	0.92	0.12	60,60,60,60	0
56	MG	1A	3147	1/1	0.92	0.18	34,34,34,34	0
56	MG	1A	3042	1/1	0.92	0.16	27,27,27,27	0
56	MG	1P	202	1/1	0.92	0.26	33,33,33,33	0
56	MG	2A	3332	1/1	0.92	0.06	37,37,37,37	0
56	MG	1A	3463	1/1	0.92	0.16	25,25,25,25	0
56	MG	2A	3060	1/1	0.92	0.12	42,42,42,42	0
56	MG	1A	3152	1/1	0.92	0.19	37,37,37,37	0
56	MG	2B	3016	1/1	0.92	0.27	66,66,66,66	0
56	MG	1A	3468	1/1	0.92	0.18	44,44,44,44	0
56	MG	1A	3004	1/1	0.92	0.17	28,28,28,28	0
56	MG	2A	3351	1/1	0.92	0.12	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	3863	1/1	0.92	0.12	31,31,31,31	0
56	MG	1A	3865	1/1	0.92	0.14	41,41,41,41	0
56	MG	1S	3001	1/1	0.92	0.47	52,52,52,52	0
56	MG	1A	3231	1/1	0.92	0.20	53,53,53,53	0
56	MG	1A	3265	1/1	0.92	0.21	40,40,40,40	0
56	MG	1W	3004	1/1	0.92	0.16	33,33,33,33	0
56	MG	1A	3203	1/1	0.92	0.14	44,44,44,44	0
56	MG	2A	3375	1/1	0.92	0.10	53,53,53,53	0
56	MG	1A	3741	1/1	0.92	0.14	58,58,58,58	0
56	MG	2Q	201	1/1	0.92	1.00	61,61,61,61	0
56	MG	2A	3381	1/1	0.92	0.19	46,46,46,46	0
56	MG	1a	1735	1/1	0.92	0.16	58,58,58,58	0
56	MG	1a	1736	1/1	0.92	0.07	58,58,58,58	0
56	MG	2X	101	1/1	0.92	0.16	37,37,37,37	0
56	MG	1a	1739	1/1	0.92	0.11	51,51,51,51	0
56	MG	2A	3088	1/1	0.92	0.17	53,53,53,53	0
56	MG	2A	3090	1/1	0.92	0.47	53,53,53,53	0
56	MG	23	3001	1/1	0.92	0.20	54,54,54,54	0
56	MG	26	502	1/1	0.92	0.14	45,45,45,45	0
56	MG	1A	3036	1/1	0.92	0.23	49,49,49,49	0
56	MG	1A	3313	1/1	0.92	0.32	41,41,41,41	0
56	MG	2a	1605	1/1	0.92	0.12	81,81,81,81	0
56	MG	2a	1606	1/1	0.92	0.12	61,61,61,61	0
56	MG	2A	3395	1/1	0.92	0.14	46,46,46,46	0
56	MG	2A	3097	1/1	0.92	0.14	57,57,57,57	0
56	MG	1A	3314	1/1	0.92	0.36	42,42,42,42	0
56	MG	1A	3101	1/1	0.92	0.29	47,47,47,47	0
56	MG	1A	3882	1/1	0.92	0.13	52,52,52,52	0
56	MG	13	103	1/1	0.92	0.15	50,50,50,50	0
56	MG	1A	3497	1/1	0.92	0.07	29,29,29,29	0
56	MG	2A	3412	1/1	0.92	0.17	40,40,40,40	0
56	MG	1A	3383	1/1	0.92	0.21	33,33,33,33	0
56	MG	1A	3625	1/1	0.92	0.10	51,51,51,51	0
56	MG	1A	3270	1/1	0.92	0.18	57,57,57,57	0
56	MG	2A	3421	1/1	0.92	0.23	52,52,52,52	0
56	MG	2A	3119	1/1	0.92	0.12	37,37,37,37	0
56	MG	2A	3121	1/1	0.92	0.16	41,41,41,41	0
56	MG	2A	3429	1/1	0.92	0.11	29,29,29,29	0
56	MG	1A	3629	1/1	0.92	0.13	42,42,42,42	0
56	MG	1A	3108	1/1	0.92	0.33	39,39,39,39	0
56	MG	1A	3325	1/1	0.92	0.15	38,38,38,38	0
56	MG	2a	1635	1/1	0.92	0.15	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	2A	3446	1/1	0.92	0.10	43,43,43,43	0
56	MG	1A	3633	1/1	0.92	0.20	40,40,40,40	0
56	MG	2a	1646	1/1	0.92	0.14	55,55,55,55	0
56	MG	2A	3464	1/1	0.92	0.09	41,41,41,41	0
56	MG	1A	3634	1/1	0.92	0.14	56,56,56,56	0
56	MG	2A	3473	1/1	0.92	0.08	51,51,51,51	0
56	MG	2a	1650	1/1	0.92	0.17	47,47,47,47	0
56	MG	2A	3136	1/1	0.92	0.20	45,45,45,45	0
56	MG	1A	3132	1/1	0.92	0.22	37,37,37,37	0
56	MG	1A	3907	1/1	0.92	0.24	40,40,40,40	0
56	MG	1a	1782	1/1	0.92	0.17	44,44,44,44	0
56	MG	2A	3487	1/1	0.92	0.09	56,56,56,56	0
56	MG	2A	3142	1/1	0.92	0.18	37,37,37,37	0
56	MG	1a	1788	1/1	0.92	0.13	64,64,64,64	0
56	MG	1A	3412	1/1	0.92	0.13	35,35,35,35	0
56	MG	1a	1790	1/1	0.92	0.13	46,46,46,46	0
56	MG	1A	3514	1/1	0.92	0.16	40,40,40,40	0
56	MG	1A	3177	1/1	0.92	0.13	44,44,44,44	0
56	MG	1A	3919	1/1	0.92	0.34	33,33,33,33	0
56	MG	2A	3170	1/1	0.92	0.13	58,58,58,58	0
56	MG	1A	3923	1/1	0.92	0.21	39,39,39,39	0
56	MG	1A	3927	1/1	0.92	0.15	40,40,40,40	0
56	MG	1A	3091	1/1	0.92	0.15	48,48,48,48	0
56	MG	1A	3523	1/1	0.92	0.15	57,57,57,57	0
56	MG	2a	1679	1/1	0.92	0.19	64,64,64,64	0
56	MG	1A	3934	1/1	0.92	0.32	30,30,30,30	0
56	MG	2a	1681	1/1	0.92	0.26	47,47,47,47	0
56	MG	2a	1685	1/1	0.92	0.11	53,53,53,53	0
56	MG	1A	3645	1/1	0.92	0.11	23,23,23,23	0
56	MG	1A	3335	1/1	0.92	0.26	47,47,47,47	0
56	MG	1a	1637	1/1	0.92	0.10	47,47,47,47	0
56	MG	1a	1639	1/1	0.92	0.18	45,45,45,45	0
56	MG	2a	1700	1/1	0.92	0.09	60,60,60,60	0
56	MG	1A	3526	1/1	0.92	0.11	49,49,49,49	0
56	MG	1A	3659	1/1	0.92	0.06	64,64,64,64	0
56	MG	2a	1707	1/1	0.92	0.07	60,60,60,60	0
56	MG	1A	3181	1/1	0.92	0.22	48,48,48,48	0
56	MG	2a	1717	1/1	0.92	0.15	59,59,59,59	0
56	MG	1A	3340	1/1	0.92	0.15	51,51,51,51	0
56	MG	1a	1647	1/1	0.92	0.16	60,60,60,60	0
56	MG	1A	3427	1/1	0.92	0.16	39,39,39,39	0
56	MG	1B	3003	1/1	0.92	0.29	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3537	1/1	0.92	0.09	57,57,57,57	0
56	MG	1A	3543	1/1	0.92	0.17	55,55,55,55	0
56	MG	1a	1652	1/1	0.92	0.11	51,51,51,51	0
56	MG	1a	1653	1/1	0.92	0.19	59,59,59,59	0
56	MG	1A	3797	1/1	0.92	0.15	57,57,57,57	0
56	MG	1A	3798	1/1	0.92	0.11	43,43,43,43	0
56	MG	2A	3549	1/1	0.92	0.21	45,45,45,45	0
56	MG	1a	1839	1/1	0.92	0.11	37,37,37,37	0
56	MG	1A	3114	1/1	0.92	0.27	32,32,32,32	0
56	MG	1d	502	1/1	0.92	0.18	51,51,51,51	0
56	MG	2a	1743	1/1	0.92	0.10	54,54,54,54	0
56	MG	2a	1747	1/1	0.92	0.22	72,72,72,72	0
56	MG	1A	3431	1/1	0.92	0.12	45,45,45,45	0
56	MG	1A	3343	1/1	0.92	0.19	54,54,54,54	0
56	MG	1v	3001	1/1	0.92	0.12	56,56,56,56	0
56	MG	1A	3560	1/1	0.92	0.16	49,49,49,49	0
56	MG	2a	1764	1/1	0.92	0.17	53,53,53,53	0
56	MG	2A	3229	1/1	0.92	0.19	53,53,53,53	0
56	MG	1A	3437	1/1	0.92	0.15	28,28,28,28	0
56	MG	1B	3016	1/1	0.92	0.19	61,61,61,61	0
56	MG	1w	3005	1/1	0.92	0.18	82,82,82,82	0
56	MG	1A	3809	1/1	0.92	0.14	42,42,42,42	0
56	MG	1a	1670	1/1	0.92	0.15	40,40,40,40	0
56	MG	1A	3691	1/1	0.92	0.17	41,41,41,41	0
56	MG	1A	3693	1/1	0.92	0.21	48,48,48,48	0
56	MG	2A	3579	1/1	0.92	0.13	65,65,65,65	0
56	MG	1B	3026	1/1	0.92	0.10	62,62,62,62	0
56	MG	2a	1786	1/1	0.92	0.10	59,59,59,59	0
56	MG	1A	3055	1/1	0.92	0.18	50,50,50,50	0
56	MG	1a	1679	1/1	0.92	0.16	48,48,48,48	0
56	MG	1A	3569	1/1	0.92	0.14	50,50,50,50	0
56	MG	2a	1794	1/1	0.92	0.13	51,51,51,51	0
56	MG	2d	302	1/1	0.92	0.21	67,67,67,67	0
56	MG	1A	3821	1/1	0.92	0.22	47,47,47,47	0
56	MG	1A	3698	1/1	0.92	0.21	43,43,43,43	0
56	MG	1A	3824	1/1	0.92	0.16	36,36,36,36	0
56	MG	1A	3570	1/1	0.92	0.14	43,43,43,43	0
56	MG	2A	3269	1/1	0.92	0.15	38,38,38,38	0
56	MG	2A	3027	1/1	0.92	0.11	44,44,44,44	0
56	MG	1A	3575	1/1	0.92	0.20	38,38,38,38	0
56	MG	1a	1690	1/1	0.92	0.14	47,47,47,47	0
56	MG	2A	3621	1/1	0.92	0.15	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3282	1/1	0.92	0.13	33,33,33,33	0
56	MG	2A	3625	1/1	0.92	0.08	56,56,56,56	0
56	MG	2A	3032	1/1	0.92	0.15	35,35,35,35	0
59	ZN	29	501	1/1	0.92	0.11	62,62,62,62	0
61	FME	1x	3011	10/11	0.92	0.32	37,40,51,79	10
56	MG	2A	3634	1/1	0.92	0.17	38,38,38,38	0
56	MG	1A	3302	1/1	0.93	0.28	30,30,30,30	0
56	MG	1A	3482	1/1	0.93	0.14	27,27,27,27	0
56	MG	1A	3869	1/1	0.93	0.13	52,52,52,52	0
56	MG	2A	3646	1/1	0.93	0.11	39,39,39,39	0
56	MG	1A	3223	1/1	0.93	0.29	42,42,42,42	0
56	MG	1A	3305	1/1	0.93	0.17	42,42,42,42	0
56	MG	1A	3190	1/1	0.93	0.19	43,43,43,43	0
56	MG	2A	3660	1/1	0.93	0.08	42,42,42,42	0
56	MG	1T	203	1/1	0.93	0.09	42,42,42,42	0
56	MG	2A	3063	1/1	0.93	0.16	43,43,43,43	0
56	MG	2A	3674	1/1	0.93	0.16	47,47,47,47	0
56	MG	2A	3675	1/1	0.93	0.26	55,55,55,55	0
56	MG	2A	3312	1/1	0.93	0.16	48,48,48,48	0
56	MG	1A	3743	1/1	0.93	0.17	38,38,38,38	0
56	MG	1A	3876	1/1	0.93	0.13	55,55,55,55	0
56	MG	1A	3619	1/1	0.93	0.20	53,53,53,53	0
56	MG	2A	3067	1/1	0.93	0.09	32,32,32,32	0
56	MG	1W	3006	1/1	0.93	0.15	46,46,46,46	0
56	MG	2A	3070	1/1	0.93	0.15	28,28,28,28	0
56	MG	2A	3071	1/1	0.93	0.42	34,34,34,34	0
56	MG	2A	3339	1/1	0.93	0.16	38,38,38,38	0
56	MG	2A	3072	1/1	0.93	0.12	40,40,40,40	0
56	MG	1A	3492	1/1	0.93	0.11	49,49,49,49	0
56	MG	1A	3159	1/1	0.93	0.30	34,34,34,34	0
56	MG	1A	3884	1/1	0.93	0.13	52,52,52,52	0
56	MG	1A	3885	1/1	0.93	0.19	44,44,44,44	0
56	MG	2A	3355	1/1	0.93	0.19	49,49,49,49	0
56	MG	2A	3078	1/1	0.93	0.14	47,47,47,47	0
56	MG	2A	3359	1/1	0.93	0.11	44,44,44,44	0
56	MG	2A	3079	1/1	0.93	0.17	49,49,49,49	0
56	MG	2A	3081	1/1	0.93	0.16	39,39,39,39	0
56	MG	1A	3193	1/1	0.93	0.19	33,33,33,33	0
56	MG	1A	3163	1/1	0.93	0.14	41,41,41,41	0
56	MG	2A	3369	1/1	0.93	0.10	50,50,50,50	0
56	MG	12	3001	1/1	0.93	0.17	53,53,53,53	0
56	MG	2A	3085	1/1	0.93	0.13	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	1A	3197	1/1	0.93	0.21	51,51,51,51	0
56	MG	1A	3390	1/1	0.93	0.15	42,42,42,42	0
56	MG	2A	3379	1/1	0.93	0.15	42,42,42,42	0
56	MG	1A	3393	1/1	0.93	0.14	35,35,35,35	0
56	MG	1a	1751	1/1	0.93	0.18	45,45,45,45	0
56	MG	2A	3092	1/1	0.93	0.15	38,38,38,38	0
56	MG	1A	3894	1/1	0.93	0.15	47,47,47,47	0
56	MG	1a	1602	1/1	0.93	0.17	68,68,68,68	0
56	MG	2a	1604	1/1	0.93	0.09	60,60,60,60	0
56	MG	2A	3390	1/1	0.93	0.11	30,30,30,30	0
56	MG	1A	3320	1/1	0.93	0.23	59,59,59,59	0
56	MG	1A	3407	1/1	0.93	0.09	34,34,34,34	0
56	MG	1A	3011	1/1	0.93	0.21	41,41,41,41	0
56	MG	2a	1612	1/1	0.93	0.14	54,54,54,54	0
56	MG	2A	3103	1/1	0.93	0.25	49,49,49,49	0
56	MG	2A	3105	1/1	0.93	0.19	49,49,49,49	0
56	MG	2A	3107	1/1	0.93	0.13	47,47,47,47	0
56	MG	1A	3638	1/1	0.93	0.18	27,27,27,27	0
56	MG	2A	3401	1/1	0.93	0.12	45,45,45,45	0
56	MG	2a	1619	1/1	0.93	0.08	46,46,46,46	0
56	MG	2A	3111	1/1	0.93	0.15	43,43,43,43	0
56	MG	1A	3411	1/1	0.93	0.15	51,51,51,51	0
56	MG	1a	1764	1/1	0.93	0.12	38,38,38,38	0
56	MG	1A	3640	1/1	0.93	0.20	21,21,21,21	0
56	MG	1a	1769	1/1	0.93	0.15	69,69,69,69	0
56	MG	1A	3059	1/1	0.93	0.18	50,50,50,50	0
56	MG	1A	3272	1/1	0.93	0.17	38,38,38,38	0
56	MG	1A	3643	1/1	0.93	0.19	30,30,30,30	0
56	MG	2A	3122	1/1	0.93	0.19	60,60,60,60	0
56	MG	2A	3123	1/1	0.93	0.26	47,47,47,47	0
56	MG	2A	3426	1/1	0.93	0.12	38,38,38,38	0
56	MG	1A	3918	1/1	0.93	0.18	35,35,35,35	0
56	MG	2a	1637	1/1	0.93	0.14	60,60,60,60	0
56	MG	1A	3039	1/1	0.93	0.26	50,50,50,50	0
56	MG	1A	3920	1/1	0.93	0.24	33,33,33,33	0
56	MG	1A	3418	1/1	0.93	0.20	34,34,34,34	0
56	MG	1a	1791	1/1	0.93	0.16	62,62,62,62	0
56	MG	2A	3133	1/1	0.93	0.17	49,49,49,49	0
56	MG	1a	1793	1/1	0.93	0.09	45,45,45,45	0
56	MG	1A	3782	1/1	0.93	0.16	34,34,34,34	0
56	MG	2A	3471	1/1	0.93	0.10	47,47,47,47	0
56	MG	1A	3647	1/1	0.93	0.07	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3206	1/1	0.93	0.15	36,36,36,36	0
56	MG	1A	3006	1/1	0.93	0.13	53,53,53,53	0
56	MG	1a	1632	1/1	0.93	0.14	54,54,54,54	0
56	MG	1A	3423	1/1	0.93	0.13	42,42,42,42	0
56	MG	1A	3540	1/1	0.93	0.14	33,33,33,33	0
56	MG	1A	3277	1/1	0.93	0.22	57,57,57,57	0
56	MG	1A	3947	1/1	0.93	0.28	49,49,49,49	0
56	MG	2a	1665	1/1	0.93	0.14	55,55,55,55	0
56	MG	2A	3168	1/1	0.93	0.20	46,46,46,46	0
56	MG	1A	3171	1/1	0.93	0.20	43,43,43,43	0
56	MG	1A	3955	1/1	0.93	0.24	29,29,29,29	0
56	MG	2A	3171	1/1	0.93	0.13	43,43,43,43	0
56	MG	1A	3958	1/1	0.93	0.73	49,49,49,49	0
56	MG	1A	3428	1/1	0.93	0.13	43,43,43,43	0
56	MG	1a	1812	1/1	0.93	0.16	51,51,51,51	0
56	MG	1a	1814	1/1	0.93	0.19	57,57,57,57	0
56	MG	1A	3961	1/1	0.93	0.34	45,45,45,45	0
56	MG	1A	3962	1/1	0.93	0.15	35,35,35,35	0
56	MG	1A	3211	1/1	0.93	0.17	38,38,38,38	0
56	MG	2A	3519	1/1	0.93	0.15	43,43,43,43	0
56	MG	2a	1687	1/1	0.93	0.12	52,52,52,52	0
56	MG	1A	3669	1/1	0.93	0.18	34,34,34,34	0
56	MG	1A	3176	1/1	0.93	0.16	27,27,27,27	0
56	MG	1A	3671	1/1	0.93	0.14	38,38,38,38	0
56	MG	1A	3281	1/1	0.93	0.14	48,48,48,48	0
56	MG	2A	3195	1/1	0.93	0.19	47,47,47,47	0
56	MG	2a	1701	1/1	0.93	0.15	62,62,62,62	0
56	MG	2a	1702	1/1	0.93	0.12	60,60,60,60	0
56	MG	2A	3525	1/1	0.93	0.10	52,52,52,52	0
56	MG	1A	3144	1/1	0.93	0.29	40,40,40,40	0
56	MG	1a	1655	1/1	0.93	0.20	63,63,63,63	0
56	MG	1A	3683	1/1	0.93	0.15	50,50,50,50	0
56	MG	2a	1715	1/1	0.93	0.29	53,53,53,53	0
56	MG	1A	3810	1/1	0.93	0.13	36,36,36,36	0
56	MG	2A	3203	1/1	0.93	0.14	40,40,40,40	0
56	MG	2A	3204	1/1	0.93	0.23	47,47,47,47	0
56	MG	1A	3284	1/1	0.93	0.22	42,42,42,42	0
56	MG	2A	3209	1/1	0.93	0.08	41,41,41,41	0
56	MG	1A	3246	1/1	0.93	0.21	48,48,48,48	0
56	MG	1A	3692	1/1	0.93	0.21	44,44,44,44	0
56	MG	2a	1728	1/1	0.93	0.13	52,52,52,52	0
56	MG	1A	3447	1/1	0.93	0.17	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	1e	201	1/1	0.93	0.30	60,60,60,60	0
56	MG	1A	3145	1/1	0.93	0.28	36,36,36,36	0
56	MG	1A	3581	1/1	0.93	0.21	50,50,50,50	0
56	MG	2A	3218	1/1	0.93	0.29	49,49,49,49	0
56	MG	1A	3582	1/1	0.93	0.16	45,45,45,45	0
56	MG	1A	3457	1/1	0.93	0.19	30,30,30,30	0
56	MG	1B	3028	1/1	0.93	0.15	39,39,39,39	0
56	MG	1A	3700	1/1	0.93	0.17	40,40,40,40	0
56	MG	2a	1745	1/1	0.93	0.20	78,78,78,78	0
56	MG	1D	304	1/1	0.93	0.19	44,44,44,44	0
56	MG	1A	3828	1/1	0.93	0.16	58,58,58,58	0
56	MG	2A	3228	1/1	0.93	0.11	43,43,43,43	0
56	MG	1x	3004	1/1	0.93	0.26	47,47,47,47	0
56	MG	2a	1759	1/1	0.93	0.10	76,76,76,76	0
56	MG	2A	3573	1/1	0.93	0.08	54,54,54,54	0
56	MG	1A	3354	1/1	0.93	0.19	45,45,45,45	0
56	MG	1x	3006	1/1	0.93	0.13	51,51,51,51	0
56	MG	1E	304	1/1	0.93	0.06	57,57,57,57	0
56	MG	1a	1683	1/1	0.93	0.25	64,64,64,64	0
56	MG	1A	3086	1/1	0.93	0.15	41,41,41,41	0
56	MG	1A	3837	1/1	0.93	0.18	21,21,21,21	0
56	MG	2A	3582	1/1	0.93	0.14	47,47,47,47	0
56	MG	2A	3006	1/1	0.93	0.13	53,53,53,53	0
56	MG	1A	3219	1/1	0.93	0.22	40,40,40,40	0
56	MG	2a	1780	1/1	0.93	0.17	64,64,64,64	0
56	MG	2A	3588	1/1	0.93	0.09	60,60,60,60	0
56	MG	1a	1688	1/1	0.93	0.12	44,44,44,44	0
56	MG	2a	1785	1/1	0.93	0.14	66,66,66,66	0
56	MG	1A	3362	1/1	0.93	0.33	36,36,36,36	0
56	MG	2a	1788	1/1	0.93	0.16	68,68,68,68	0
56	MG	1A	3714	1/1	0.93	0.13	48,48,48,48	0
56	MG	2A	3601	1/1	0.93	0.14	49,49,49,49	0
56	MG	1A	3052	1/1	0.93	0.21	39,39,39,39	0
56	MG	1A	3365	1/1	0.93	0.17	48,48,48,48	0
56	MG	2A	3605	1/1	0.93	0.11	45,45,45,45	0
56	MG	1A	3090	1/1	0.93	0.18	39,39,39,39	0
56	MG	1O	202	1/1	0.93	0.22	63,63,63,63	0
56	MG	2A	3255	1/1	0.93	0.15	43,43,43,43	0
56	MG	2A	3256	1/1	0.93	0.11	33,33,33,33	0
56	MG	2A	3261	1/1	0.93	0.19	34,34,34,34	0
56	MG	2A	3266	1/1	0.93	0.14	34,34,34,34	0
56	MG	2v	3001	1/1	0.93	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	1A	3719	1/1	0.93	0.17	41,41,41,41	0
56	MG	1A	3368	1/1	0.93	0.14	41,41,41,41	0
56	MG	2A	3626	1/1	0.93	0.12	49,49,49,49	0
56	MG	2x	101	1/1	0.93	0.22	56,56,56,56	0
56	MG	1a	1700	1/1	0.93	0.28	51,51,51,51	0
57	K	1A	3321	1/1	0.93	0.14	84,84,84,84	0
56	MG	2A	3276	1/1	0.93	0.09	48,48,48,48	0
56	MG	1A	3859	1/1	0.93	0.14	53,53,53,53	0
56	MG	1A	3112	1/1	0.93	0.26	43,43,43,43	0
59	ZN	2n	501	1/1	0.93	0.08	108,108,108,108	0
56	MG	1A	3476	1/1	0.93	0.07	31,31,31,31	0
56	MG	1A	3477	1/1	0.93	0.17	23,23,23,23	0
56	MG	1A	3628	1/1	0.94	0.19	47,47,47,47	0
56	MG	1A	3209	1/1	0.94	0.16	35,35,35,35	0
56	MG	1A	3329	1/1	0.94	0.20	38,38,38,38	0
56	MG	2A	3192	1/1	0.94	0.21	51,51,51,51	0
56	MG	1A	3501	1/1	0.94	0.18	32,32,32,32	0
56	MG	1A	3331	1/1	0.94	0.25	53,53,53,53	0
56	MG	1a	1813	1/1	0.94	0.14	72,72,72,72	0
56	MG	1A	3768	1/1	0.94	0.23	50,50,50,50	0
56	MG	1A	3769	1/1	0.94	0.43	39,39,39,39	0
56	MG	1A	3332	1/1	0.94	0.17	31,31,31,31	0
56	MG	1a	1628	1/1	0.94	0.14	43,43,43,43	0
56	MG	2A	3206	1/1	0.94	0.23	38,38,38,38	0
56	MG	1a	1824	1/1	0.94	0.17	48,48,48,48	0
56	MG	2A	3580	1/1	0.94	0.12	38,38,38,38	0
56	MG	1A	3029	1/1	0.94	0.23	28,28,28,28	0
56	MG	2A	3583	1/1	0.94	0.13	41,41,41,41	0
56	MG	1A	3087	1/1	0.94	0.14	20,20,20,20	0
56	MG	1A	3510	1/1	0.94	0.17	25,25,25,25	0
56	MG	2A	3587	1/1	0.94	0.17	48,48,48,48	0
56	MG	2A	3213	1/1	0.94	0.14	45,45,45,45	0
56	MG	1A	3180	1/1	0.94	0.13	56,56,56,56	0
56	MG	1A	3415	1/1	0.94	0.16	28,28,28,28	0
56	MG	1a	1832	1/1	0.94	0.10	47,47,47,47	0
56	MG	2A	3599	1/1	0.94	0.14	54,54,54,54	0
56	MG	1a	1833	1/1	0.94	0.27	52,52,52,52	0
56	MG	2A	3602	1/1	0.94	0.07	50,50,50,50	0
56	MG	1A	3935	1/1	0.94	0.32	48,48,48,48	0
56	MG	2A	3220	1/1	0.94	0.20	55,55,55,55	0
56	MG	1A	3148	1/1	0.94	0.32	31,31,31,31	0
56	MG	2A	3608	1/1	0.94	0.14	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3939	1/1	0.94	0.31	42,42,42,42	0
56	MG	1a	1838	1/1	0.94	0.10	51,51,51,51	0
56	MG	1A	3780	1/1	0.94	0.16	26,26,26,26	0
56	MG	1A	3519	1/1	0.94	0.08	41,41,41,41	0
56	MG	2A	3618	1/1	0.94	0.12	44,44,44,44	0
56	MG	1A	3946	1/1	0.94	0.21	38,38,38,38	0
56	MG	1A	3100	1/1	0.94	0.10	57,57,57,57	0
56	MG	1a	1646	1/1	0.94	0.19	25,25,25,25	0
56	MG	2A	3624	1/1	0.94	0.08	44,44,44,44	0
56	MG	1A	3050	1/1	0.94	0.21	46,46,46,46	0
56	MG	1A	3952	1/1	0.94	0.23	33,33,33,33	0
56	MG	2A	3627	1/1	0.94	0.11	56,56,56,56	0
56	MG	2A	3628	1/1	0.94	0.16	46,46,46,46	0
56	MG	2A	3232	1/1	0.94	0.12	41,41,41,41	0
56	MG	1w	3001	1/1	0.94	0.10	44,44,44,44	0
56	MG	1A	3524	1/1	0.94	0.16	50,50,50,50	0
56	MG	2A	3637	1/1	0.94	0.13	41,41,41,41	0
56	MG	2A	3235	1/1	0.94	0.20	49,49,49,49	0
56	MG	1A	3218	1/1	0.94	0.12	51,51,51,51	0
56	MG	1A	3250	1/1	0.94	0.36	30,30,30,30	0
56	MG	1A	3424	1/1	0.94	0.18	14,14,14,14	0
56	MG	2A	3240	1/1	0.94	0.12	46,46,46,46	0
56	MG	1w	3006	1/1	0.94	0.06	67,67,67,67	0
56	MG	2A	3242	1/1	0.94	0.13	54,54,54,54	0
56	MG	1A	3651	1/1	0.94	0.13	41,41,41,41	0
56	MG	1A	3251	1/1	0.94	0.29	25,25,25,25	0
56	MG	1A	3531	1/1	0.94	0.14	53,53,53,53	0
56	MG	2A	3247	1/1	0.94	0.12	51,51,51,51	0
56	MG	1A	3286	1/1	0.94	0.40	41,41,41,41	0
56	MG	1a	1660	1/1	0.94	0.14	47,47,47,47	0
56	MG	1B	3004	1/1	0.94	0.22	68,68,68,68	0
56	MG	1A	3534	1/1	0.94	0.08	47,47,47,47	0
56	MG	1x	3010	1/1	0.94	0.07	74,74,74,74	0
56	MG	2A	3001	1/1	0.94	0.16	28,28,28,28	0
56	MG	2A	3259	1/1	0.94	0.15	43,43,43,43	0
56	MG	2A	3260	1/1	0.94	0.10	52,52,52,52	0
56	MG	1A	3103	1/1	0.94	0.18	36,36,36,36	0
56	MG	2A	3263	1/1	0.94	0.17	45,45,45,45	0
56	MG	2B	3013	1/1	0.94	0.16	45,45,45,45	0
56	MG	2A	3003	1/1	0.94	0.10	43,43,43,43	0
56	MG	1A	3542	1/1	0.94	0.14	52,52,52,52	0
56	MG	2B	3018	1/1	0.94	0.06	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3351	1/1	0.94	0.09	51,51,51,51	0
56	MG	2A	3009	1/1	0.94	0.13	41,41,41,41	0
56	MG	2A	3272	1/1	0.94	0.15	42,42,42,42	0
56	MG	2A	3274	1/1	0.94	0.15	48,48,48,48	0
56	MG	1A	3289	1/1	0.94	0.13	29,29,29,29	0
56	MG	1A	3554	1/1	0.94	0.26	32,32,32,32	0
56	MG	2A	3014	1/1	0.94	0.12	38,38,38,38	0
56	MG	2A	3019	1/1	0.94	0.17	52,52,52,52	0
56	MG	2A	3023	1/1	0.94	0.61	49,49,49,49	0
56	MG	2A	3292	1/1	0.94	0.15	45,45,45,45	0
56	MG	2A	3293	1/1	0.94	0.08	33,33,33,33	0
56	MG	1a	1671	1/1	0.94	0.18	42,42,42,42	0
56	MG	1A	3673	1/1	0.94	0.12	59,59,59,59	0
56	MG	1B	3013	1/1	0.94	0.09	53,53,53,53	0
56	MG	1a	1674	1/1	0.94	0.13	42,42,42,42	0
56	MG	1A	3812	1/1	0.94	0.14	41,41,41,41	0
56	MG	2A	3303	1/1	0.94	0.21	60,60,60,60	0
56	MG	2Z	8001	1/1	0.94	0.13	70,70,70,70	0
56	MG	1A	3353	1/1	0.94	0.26	36,36,36,36	0
56	MG	2A	3306	1/1	0.94	0.10	33,33,33,33	0
56	MG	2A	3307	1/1	0.94	0.14	31,31,31,31	0
56	MG	1A	3816	1/1	0.94	0.47	62,62,62,62	0
56	MG	1A	3556	1/1	0.94	0.14	43,43,43,43	0
56	MG	2A	3311	1/1	0.94	0.18	45,45,45,45	0
56	MG	1A	3681	1/1	0.94	0.11	32,32,32,32	0
56	MG	1A	3557	1/1	0.94	0.11	44,44,44,44	0
56	MG	2A	3316	1/1	0.94	0.17	25,25,25,25	0
56	MG	1A	3130	1/1	0.94	0.12	50,50,50,50	0
56	MG	2a	1607	1/1	0.94	0.18	48,48,48,48	0
56	MG	2A	3044	1/1	0.94	0.16	36,36,36,36	0
56	MG	2a	1609	1/1	0.94	0.08	60,60,60,60	0
56	MG	1A	3689	1/1	0.94	0.16	35,35,35,35	0
56	MG	2A	3047	1/1	0.94	0.10	22,22,22,22	0
56	MG	2A	3048	1/1	0.94	0.55	44,44,44,44	0
56	MG	2A	3049	1/1	0.94	0.12	42,42,42,42	0
56	MG	2A	3334	1/1	0.94	0.12	44,44,44,44	0
56	MG	2A	3050	1/1	0.94	0.18	43,43,43,43	0
56	MG	2A	3340	1/1	0.94	0.10	27,27,27,27	0
56	MG	1D	302	1/1	0.94	0.18	21,21,21,21	0
56	MG	1A	3438	1/1	0.94	0.14	30,30,30,30	0
56	MG	1A	3562	1/1	0.94	0.10	42,42,42,42	0
56	MG	1A	3439	1/1	0.94	0.16	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	1A	3107	1/1	0.94	0.12	26,26,26,26	0
56	MG	2A	3353	1/1	0.94	0.10	49,49,49,49	0
56	MG	2A	3057	1/1	0.94	0.22	57,57,57,57	0
56	MG	1A	3359	1/1	0.94	0.09	44,44,44,44	0
56	MG	1A	3082	1/1	0.94	0.16	41,41,41,41	0
56	MG	2A	3360	1/1	0.94	0.09	35,35,35,35	0
56	MG	1A	3194	1/1	0.94	0.18	38,38,38,38	0
56	MG	1A	3839	1/1	0.94	0.12	70,70,70,70	0
56	MG	2A	3365	1/1	0.94	0.09	29,29,29,29	0
56	MG	1A	3455	1/1	0.94	0.14	45,45,45,45	0
56	MG	2a	1639	1/1	0.94	0.17	52,52,52,52	0
56	MG	2A	3367	1/1	0.94	0.22	42,42,42,42	0
56	MG	1a	1699	1/1	0.94	0.08	46,46,46,46	0
56	MG	1G	201	1/1	0.94	0.10	37,37,37,37	0
56	MG	2A	3370	1/1	0.94	0.11	42,42,42,42	0
56	MG	1A	3261	1/1	0.94	0.75	51,51,51,51	0
56	MG	1A	3846	1/1	0.94	0.17	51,51,51,51	0
56	MG	1N	3002	1/1	0.94	0.25	49,49,49,49	0
56	MG	1A	3703	1/1	0.94	0.10	50,50,50,50	0
56	MG	1A	3704	1/1	0.94	0.10	43,43,43,43	0
56	MG	1A	3458	1/1	0.94	0.19	42,42,42,42	0
56	MG	2a	1654	1/1	0.94	0.13	64,64,64,64	0
56	MG	1a	1709	1/1	0.94	0.22	60,60,60,60	0
56	MG	1A	3031	1/1	0.94	0.14	31,31,31,31	0
56	MG	2A	3076	1/1	0.94	0.21	31,31,31,31	0
56	MG	1A	3366	1/1	0.94	0.14	61,61,61,61	0
56	MG	2A	3389	1/1	0.94	0.24	52,52,52,52	0
56	MG	1a	1715	1/1	0.94	0.13	51,51,51,51	0
56	MG	1A	3853	1/1	0.94	0.07	41,41,41,41	0
56	MG	1A	3857	1/1	0.94	0.11	39,39,39,39	0
56	MG	1a	1719	1/1	0.94	0.14	45,45,45,45	0
56	MG	1A	3710	1/1	0.94	0.10	43,43,43,43	0
56	MG	1a	1723	1/1	0.94	0.12	62,62,62,62	0
56	MG	1A	3167	1/1	0.94	0.38	42,42,42,42	0
56	MG	1Q	202	1/1	0.94	0.26	41,41,41,41	0
56	MG	1A	3198	1/1	0.94	0.29	34,34,34,34	0
56	MG	2a	1675	1/1	0.94	0.05	66,66,66,66	0
56	MG	1a	1729	1/1	0.94	0.16	53,53,53,53	0
56	MG	1a	1730	1/1	0.94	0.22	71,71,71,71	0
56	MG	2A	3405	1/1	0.94	0.21	49,49,49,49	0
56	MG	1A	3307	1/1	0.94	0.17	55,55,55,55	0
56	MG	2a	1682	1/1	0.94	0.29	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3408	1/1	0.94	0.08	50,50,50,50	0
56	MG	2a	1686	1/1	0.94	0.32	66,66,66,66	0
56	MG	2A	3093	1/1	0.94	0.11	51,51,51,51	0
56	MG	2a	1688	1/1	0.94	0.17	56,56,56,56	0
56	MG	1A	3595	1/1	0.94	0.20	26,26,26,26	0
56	MG	2a	1690	1/1	0.94	0.26	50,50,50,50	0
56	MG	2a	1691	1/1	0.94	0.14	57,57,57,57	0
56	MG	1A	3061	1/1	0.94	0.20	36,36,36,36	0
56	MG	1A	3371	1/1	0.94	0.21	56,56,56,56	0
56	MG	1a	1738	1/1	0.94	0.05	43,43,43,43	0
56	MG	2A	3101	1/1	0.94	0.21	53,53,53,53	0
56	MG	1T	201	1/1	0.94	0.19	43,43,43,43	0
56	MG	1a	1741	1/1	0.94	0.11	47,47,47,47	0
56	MG	1A	3229	1/1	0.94	0.15	40,40,40,40	0
56	MG	1U	202	1/1	0.94	0.13	31,31,31,31	0
56	MG	2A	3109	1/1	0.94	0.09	49,49,49,49	0
56	MG	1U	204	1/1	0.94	0.20	44,44,44,44	0
56	MG	2a	1711	1/1	0.94	0.18	57,57,57,57	0
56	MG	2a	1714	1/1	0.94	0.12	55,55,55,55	0
56	MG	2A	3442	1/1	0.94	0.08	46,46,46,46	0
56	MG	2a	1716	1/1	0.94	0.07	52,52,52,52	0
56	MG	1A	3137	1/1	0.94	0.21	32,32,32,32	0
56	MG	1a	1747	1/1	0.94	0.17	55,55,55,55	0
56	MG	2A	3452	1/1	0.94	0.30	54,54,54,54	0
56	MG	1A	3016	1/1	0.94	0.12	34,34,34,34	0
56	MG	2A	3465	1/1	0.94	0.12	39,39,39,39	0
56	MG	1W	3002	1/1	0.94	0.17	49,49,49,49	0
56	MG	2A	3470	1/1	0.94	0.13	30,30,30,30	0
56	MG	2a	1726	1/1	0.94	0.11	64,64,64,64	0
56	MG	1A	3603	1/1	0.94	0.13	31,31,31,31	0
56	MG	1A	3232	1/1	0.94	0.12	49,49,49,49	0
56	MG	1X	3002	1/1	0.94	0.17	45,45,45,45	0
56	MG	2A	3475	1/1	0.94	0.06	52,52,52,52	0
56	MG	2A	3120	1/1	0.94	0.10	53,53,53,53	0
56	MG	2A	3480	1/1	0.94	0.19	72,72,72,72	0
56	MG	2A	3481	1/1	0.94	0.24	58,58,58,58	0
56	MG	1X	3004	1/1	0.94	0.27	64,64,64,64	0
56	MG	1A	3479	1/1	0.94	0.19	48,48,48,48	0
56	MG	2a	1742	1/1	0.94	0.16	62,62,62,62	0
56	MG	2A	3485	1/1	0.94	0.10	59,59,59,59	0
56	MG	1A	3480	1/1	0.94	0.16	26,26,26,26	0
56	MG	2A	3489	1/1	0.94	0.12	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3124	1/1	0.94	0.10	50,50,50,50	0
56	MG	1A	3881	1/1	0.94	0.10	48,48,48,48	0
56	MG	1A	3175	1/1	0.94	0.15	31,31,31,31	0
56	MG	2a	1757	1/1	0.94	0.10	70,70,70,70	0
56	MG	2A	3494	1/1	0.94	0.14	45,45,45,45	0
56	MG	1A	3883	1/1	0.94	0.08	60,60,60,60	0
56	MG	2a	1762	1/1	0.94	0.13	55,55,55,55	0
56	MG	1a	1766	1/1	0.94	0.16	59,59,59,59	0
56	MG	2A	3130	1/1	0.94	0.30	54,54,54,54	0
56	MG	1A	3115	1/1	0.94	0.12	37,37,37,37	0
56	MG	10	103	1/1	0.94	0.10	60,60,60,60	0
56	MG	2A	3503	1/1	0.94	0.11	47,47,47,47	0
56	MG	2A	3135	1/1	0.94	0.17	33,33,33,33	0
56	MG	2A	3506	1/1	0.94	0.12	50,50,50,50	0
56	MG	1A	3746	1/1	0.94	0.07	45,45,45,45	0
56	MG	1A	3323	1/1	0.94	0.26	50,50,50,50	0
56	MG	2A	3138	1/1	0.94	0.14	47,47,47,47	0
56	MG	1A	3748	1/1	0.94	0.13	29,29,29,29	0
56	MG	1a	1778	1/1	0.94	0.14	66,66,66,66	0
56	MG	16	502	1/1	0.94	0.19	51,51,51,51	0
56	MG	2A	3144	1/1	0.94	0.13	43,43,43,43	0
56	MG	2A	3149	1/1	0.94	0.13	49,49,49,49	0
56	MG	1a	1783	1/1	0.94	0.12	63,63,63,63	0
56	MG	1a	1784	1/1	0.94	0.08	58,58,58,58	0
56	MG	2A	3160	1/1	0.94	0.12	47,47,47,47	0
56	MG	2a	1792	1/1	0.94	0.15	50,50,50,50	0
56	MG	2a	1793	1/1	0.94	0.13	41,41,41,41	0
56	MG	17	101	1/1	0.94	0.27	48,48,48,48	0
56	MG	2a	1795	1/1	0.94	0.07	55,55,55,55	0
56	MG	2a	1796	1/1	0.94	0.15	60,60,60,60	0
56	MG	1A	3889	1/1	0.94	0.13	36,36,36,36	0
56	MG	1A	3749	1/1	0.94	0.14	52,52,52,52	0
56	MG	2g	8001	1/1	0.94	0.10	57,57,57,57	0
56	MG	2A	3531	1/1	0.94	0.18	45,45,45,45	0
56	MG	19	102	1/1	0.94	0.12	50,50,50,50	0
56	MG	1a	1601	1/1	0.94	0.14	53,53,53,53	0
56	MG	1A	3388	1/1	0.94	0.12	49,49,49,49	0
56	MG	1A	3488	1/1	0.94	0.19	28,28,28,28	0
56	MG	1A	3389	1/1	0.94	0.14	50,50,50,50	0
56	MG	1a	1605	1/1	0.94	0.11	50,50,50,50	0
56	MG	2A	3175	1/1	0.94	0.24	54,54,54,54	0
56	MG	1A	3274	1/1	0.94	0.28	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3392	1/1	0.94	0.19	39,39,39,39	0
56	MG	1A	3759	1/1	0.94	0.17	45,45,45,45	0
56	MG	2A	3181	1/1	0.94	0.11	44,44,44,44	0
56	MG	1A	3902	1/1	0.94	0.17	28,28,28,28	0
59	ZN	14	501	1/1	0.94	0.07	97,97,97,97	0
56	MG	2A	3553	1/1	0.94	0.06	53,53,53,53	0
56	MG	2A	3554	1/1	0.94	0.07	45,45,45,45	0
56	MG	1a	1804	1/1	0.94	0.09	65,65,65,65	0
56	MG	2A	3557	1/1	0.94	0.14	49,49,49,49	0
56	MG	1A	3627	1/1	0.94	0.07	44,44,44,44	0
56	MG	1A	3873	1/1	0.95	0.15	39,39,39,39	0
56	MG	2A	3304	1/1	0.95	0.23	53,53,53,53	0
56	MG	2A	3623	1/1	0.95	0.09	46,46,46,46	0
56	MG	1A	3725	1/1	0.95	0.15	28,28,28,28	0
56	MG	1A	3604	1/1	0.95	0.25	29,29,29,29	0
56	MG	1A	3495	1/1	0.95	0.20	43,43,43,43	0
56	MG	1A	3730	1/1	0.95	0.12	47,47,47,47	0
56	MG	1A	3607	1/1	0.95	0.21	30,30,30,30	0
56	MG	2A	3631	1/1	0.95	0.14	51,51,51,51	0
56	MG	1A	3168	1/1	0.95	0.23	47,47,47,47	0
56	MG	2A	3633	1/1	0.95	0.11	49,49,49,49	0
56	MG	1A	3416	1/1	0.95	0.14	54,54,54,54	0
56	MG	1A	3739	1/1	0.95	0.09	48,48,48,48	0
56	MG	1A	3125	1/1	0.95	0.32	36,36,36,36	0
56	MG	2A	3319	1/1	0.95	0.16	29,29,29,29	0
56	MG	1a	1749	1/1	0.95	0.09	56,56,56,56	0
56	MG	2A	3321	1/1	0.95	0.24	53,53,53,53	0
56	MG	1A	3611	1/1	0.95	0.18	46,46,46,46	0
56	MG	2A	3324	1/1	0.95	0.15	50,50,50,50	0
56	MG	1A	3350	1/1	0.95	0.15	44,44,44,44	0
56	MG	1A	3745	1/1	0.95	0.14	61,61,61,61	0
56	MG	2A	3648	1/1	0.95	0.27	47,47,47,47	0
56	MG	11	101	1/1	0.95	0.07	41,41,41,41	0
56	MG	11	103	1/1	0.95	0.25	45,45,45,45	0
56	MG	1A	3003	1/1	0.95	0.14	32,32,32,32	0
56	MG	2A	3657	1/1	0.95	0.06	36,36,36,36	0
56	MG	2A	3658	1/1	0.95	0.11	39,39,39,39	0
56	MG	1A	3616	1/1	0.95	0.22	55,55,55,55	0
56	MG	2A	3091	1/1	0.95	0.18	29,29,29,29	0
56	MG	1A	3504	1/1	0.95	0.17	50,50,50,50	0
56	MG	2A	3669	1/1	0.95	0.33	44,44,44,44	0
56	MG	1a	1760	1/1	0.95	0.17	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	3420	1/1	0.95	0.08	59,59,59,59	0
56	MG	1a	1763	1/1	0.95	0.07	56,56,56,56	0
56	MG	2A	3348	1/1	0.95	0.17	55,55,55,55	0
56	MG	1A	3623	1/1	0.95	0.18	53,53,53,53	0
56	MG	2B	3004	1/1	0.95	0.23	62,62,62,62	0
56	MG	2A	3099	1/1	0.95	0.15	24,24,24,24	0
56	MG	2B	3007	1/1	0.95	0.13	46,46,46,46	0
56	MG	1A	3291	1/1	0.95	0.27	28,28,28,28	0
56	MG	1A	3508	1/1	0.95	0.17	38,38,38,38	0
56	MG	2B	3010	1/1	0.95	0.10	50,50,50,50	0
56	MG	1A	3899	1/1	0.95	0.18	14,14,14,14	0
56	MG	1a	1771	1/1	0.95	0.10	54,54,54,54	0
56	MG	1A	3756	1/1	0.95	0.14	39,39,39,39	0
56	MG	2B	3017	1/1	0.95	0.31	63,63,63,63	0
56	MG	1A	3066	1/1	0.95	0.39	31,31,31,31	0
56	MG	2A	3108	1/1	0.95	0.15	30,30,30,30	0
56	MG	1A	3173	1/1	0.95	0.22	36,36,36,36	0
56	MG	1a	1777	1/1	0.95	0.14	47,47,47,47	0
56	MG	1A	3068	1/1	0.95	0.18	43,43,43,43	0
56	MG	1a	1779	1/1	0.95	0.14	36,36,36,36	0
56	MG	2E	304	1/1	0.95	0.12	47,47,47,47	0
56	MG	1A	3256	1/1	0.95	0.14	49,49,49,49	0
56	MG	2A	3114	1/1	0.95	0.24	51,51,51,51	0
56	MG	1A	3518	1/1	0.95	0.17	40,40,40,40	0
56	MG	2A	3374	1/1	0.95	0.17	54,54,54,54	0
56	MG	1A	3014	1/1	0.95	0.18	32,32,32,32	0
56	MG	1A	3913	1/1	0.95	0.15	39,39,39,39	0
56	MG	2A	3377	1/1	0.95	0.08	43,43,43,43	0
56	MG	2A	3378	1/1	0.95	0.16	48,48,48,48	0
56	MG	1A	3521	1/1	0.95	0.11	35,35,35,35	0
56	MG	2U	201	1/1	0.95	0.17	39,39,39,39	0
56	MG	2A	3380	1/1	0.95	0.09	35,35,35,35	0
56	MG	1A	3917	1/1	0.95	0.56	40,40,40,40	0
56	MG	1A	3104	1/1	0.95	0.15	33,33,33,33	0
56	MG	1a	1792	1/1	0.95	0.11	75,75,75,75	0
56	MG	1A	3105	1/1	0.95	0.20	31,31,31,31	0
56	MG	1a	1614	1/1	0.95	0.19	37,37,37,37	0
56	MG	1a	1615	1/1	0.95	0.11	65,65,65,65	0
56	MG	1A	3073	1/1	0.95	0.22	29,29,29,29	0
56	MG	1A	3435	1/1	0.95	0.14	35,35,35,35	0
56	MG	2A	3392	1/1	0.95	0.17	55,55,55,55	0
56	MG	1A	3436	1/1	0.95	0.15	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3930	1/1	0.95	0.52	36,36,36,36	0
56	MG	1A	3771	1/1	0.95	0.20	39,39,39,39	0
56	MG	1a	1623	1/1	0.95	0.14	59,59,59,59	0
56	MG	2A	3134	1/1	0.95	0.09	44,44,44,44	0
56	MG	1a	1803	1/1	0.95	0.06	64,64,64,64	0
56	MG	1A	3772	1/1	0.95	0.27	29,29,29,29	0
56	MG	1a	1805	1/1	0.95	0.16	49,49,49,49	0
56	MG	1a	1626	1/1	0.95	0.28	45,45,45,45	0
56	MG	1a	1627	1/1	0.95	0.20	58,58,58,58	0
56	MG	2A	3406	1/1	0.95	0.17	47,47,47,47	0
56	MG	1A	3139	1/1	0.95	0.17	33,33,33,33	0
56	MG	1A	3310	1/1	0.95	0.13	54,54,54,54	0
56	MG	1A	3142	1/1	0.95	0.26	17,17,17,17	0
56	MG	2A	3145	1/1	0.95	0.10	35,35,35,35	0
56	MG	1a	1811	1/1	0.95	0.22	57,57,57,57	0
56	MG	1a	1631	1/1	0.95	0.14	59,59,59,59	0
56	MG	2A	3418	1/1	0.95	0.17	44,44,44,44	0
56	MG	2A	3419	1/1	0.95	0.14	37,37,37,37	0
56	MG	2A	3151	1/1	0.95	0.19	31,31,31,31	0
56	MG	1A	3026	1/1	0.95	0.19	29,29,29,29	0
56	MG	2A	3159	1/1	0.95	0.23	41,41,41,41	0
56	MG	1A	3185	1/1	0.95	0.20	50,50,50,50	0
56	MG	1A	3535	1/1	0.95	0.18	45,45,45,45	0
56	MG	1a	1816	1/1	0.95	0.17	49,49,49,49	0
56	MG	2A	3435	1/1	0.95	0.14	43,43,43,43	0
56	MG	2A	3165	1/1	0.95	0.21	36,36,36,36	0
56	MG	2A	3440	1/1	0.95	0.20	42,42,42,42	0
56	MG	1a	1818	1/1	0.95	0.21	55,55,55,55	0
56	MG	2a	1641	1/1	0.95	0.11	65,65,65,65	0
56	MG	1A	3646	1/1	0.95	0.24	36,36,36,36	0
56	MG	1A	3537	1/1	0.95	0.14	40,40,40,40	0
56	MG	2A	3447	1/1	0.95	0.07	46,46,46,46	0
56	MG	1a	1821	1/1	0.95	0.09	68,68,68,68	0
56	MG	1a	1823	1/1	0.95	0.10	58,58,58,58	0
56	MG	2A	3456	1/1	0.95	0.16	39,39,39,39	0
56	MG	2A	3461	1/1	0.95	0.17	39,39,39,39	0
56	MG	2A	3462	1/1	0.95	0.13	57,57,57,57	0
56	MG	1a	1638	1/1	0.95	0.24	42,42,42,42	0
56	MG	1A	3111	1/1	0.95	0.15	40,40,40,40	0
56	MG	2A	3466	1/1	0.95	0.11	50,50,50,50	0
56	MG	2A	3467	1/1	0.95	0.09	65,65,65,65	0
56	MG	2a	1656	1/1	0.95	0.16	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3468	1/1	0.95	0.10	38,38,38,38	0
56	MG	1a	1640	1/1	0.95	0.21	41,41,41,41	0
56	MG	1A	3950	1/1	0.95	0.16	35,35,35,35	0
56	MG	2a	1660	1/1	0.95	0.09	61,61,61,61	0
56	MG	1A	3449	1/1	0.95	0.21	37,37,37,37	0
56	MG	1a	1643	1/1	0.95	0.33	51,51,51,51	0
56	MG	1A	3953	1/1	0.95	0.19	48,48,48,48	0
56	MG	2a	1666	1/1	0.95	0.13	49,49,49,49	0
56	MG	1A	3787	1/1	0.95	0.09	34,34,34,34	0
56	MG	1A	3188	1/1	0.95	0.13	39,39,39,39	0
56	MG	2a	1669	1/1	0.95	0.16	44,44,44,44	0
56	MG	2A	3186	1/1	0.95	0.19	43,43,43,43	0
56	MG	1A	3544	1/1	0.95	0.09	54,54,54,54	0
56	MG	1A	3546	1/1	0.95	0.13	45,45,45,45	0
56	MG	1A	3227	1/1	0.95	0.10	42,42,42,42	0
56	MG	2A	3484	1/1	0.95	0.11	53,53,53,53	0
56	MG	1A	3963	1/1	0.95	0.18	34,34,34,34	0
56	MG	2a	1677	1/1	0.95	0.18	51,51,51,51	0
56	MG	2A	3486	1/1	0.95	0.06	54,54,54,54	0
56	MG	1b	3001	1/1	0.95	0.10	75,75,75,75	0
56	MG	2A	3488	1/1	0.95	0.10	52,52,52,52	0
56	MG	2A	3194	1/1	0.95	0.21	40,40,40,40	0
56	MG	2A	3490	1/1	0.95	0.22	48,48,48,48	0
56	MG	2a	1683	1/1	0.95	0.25	57,57,57,57	0
56	MG	2a	1684	1/1	0.95	0.31	48,48,48,48	0
56	MG	1A	3553	1/1	0.95	0.14	28,28,28,28	0
56	MG	1A	3028	1/1	0.95	0.17	20,20,20,20	0
56	MG	1A	3666	1/1	0.95	0.28	44,44,44,44	0
56	MG	1A	3379	1/1	0.95	0.18	52,52,52,52	0
56	MG	1f	3001	1/1	0.95	0.18	38,38,38,38	0
56	MG	2A	3496	1/1	0.95	0.13	53,53,53,53	0
56	MG	1A	3668	1/1	0.95	0.20	35,35,35,35	0
56	MG	1A	3801	1/1	0.95	0.24	45,45,45,45	0
56	MG	1A	3191	1/1	0.95	0.06	38,38,38,38	0
56	MG	1A	3381	1/1	0.95	0.23	57,57,57,57	0
56	MG	2a	1698	1/1	0.95	0.16	57,57,57,57	0
56	MG	1B	3009	1/1	0.95	0.19	42,42,42,42	0
56	MG	1A	3326	1/1	0.95	0.23	43,43,43,43	0
56	MG	1A	3559	1/1	0.95	0.07	41,41,41,41	0
56	MG	2a	1703	1/1	0.95	0.18	61,61,61,61	0
56	MG	1A	3007	1/1	0.95	0.21	29,29,29,29	0
56	MG	2a	1705	1/1	0.95	0.12	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	2A	3510	1/1	0.95	0.11	31,31,31,31	0
56	MG	2A	3511	1/1	0.95	0.11	68,68,68,68	0
56	MG	1A	3675	1/1	0.95	0.17	56,56,56,56	0
56	MG	1A	3464	1/1	0.95	0.16	35,35,35,35	0
56	MG	1A	3813	1/1	0.95	0.31	40,40,40,40	0
56	MG	2A	3518	1/1	0.95	0.07	50,50,50,50	0
56	MG	1A	3679	1/1	0.95	0.15	52,52,52,52	0
56	MG	1A	3563	1/1	0.95	0.09	33,33,33,33	0
56	MG	1A	3092	1/1	0.95	0.16	41,41,41,41	0
56	MG	1A	3818	1/1	0.95	0.16	30,30,30,30	0
56	MG	1B	3027	1/1	0.95	0.16	48,48,48,48	0
56	MG	1A	3685	1/1	0.95	0.14	26,26,26,26	0
56	MG	2a	1723	1/1	0.95	0.07	54,54,54,54	0
56	MG	1a	1680	1/1	0.95	0.22	56,56,56,56	0
56	MG	1A	3466	1/1	0.95	0.11	50,50,50,50	0
56	MG	2A	3528	1/1	0.95	0.10	55,55,55,55	0
56	MG	2a	1727	1/1	0.95	0.09	62,62,62,62	0
56	MG	1A	3822	1/1	0.95	0.08	52,52,52,52	0
56	MG	1A	3687	1/1	0.95	0.20	39,39,39,39	0
56	MG	2A	3007	1/1	0.95	0.12	38,38,38,38	0
56	MG	1A	3568	1/1	0.95	0.21	53,53,53,53	0
56	MG	2a	1733	1/1	0.95	0.16	61,61,61,61	0
56	MG	1A	3009	1/1	0.95	0.12	30,30,30,30	0
56	MG	2A	3534	1/1	0.95	0.06	62,62,62,62	0
56	MG	2a	1737	1/1	0.95	0.22	51,51,51,51	0
56	MG	1A	3233	1/1	0.95	0.39	35,35,35,35	0
56	MG	2A	3013	1/1	0.95	0.12	36,36,36,36	0
56	MG	1A	3094	1/1	0.95	0.26	58,58,58,58	0
56	MG	1A	3829	1/1	0.95	0.24	59,59,59,59	0
56	MG	1A	3694	1/1	0.95	0.17	47,47,47,47	0
56	MG	2A	3545	1/1	0.95	0.24	47,47,47,47	0
56	MG	1A	3831	1/1	0.95	0.24	62,62,62,62	0
56	MG	1A	3577	1/1	0.95	0.18	47,47,47,47	0
56	MG	2a	1751	1/1	0.95	0.15	65,65,65,65	0
56	MG	2a	1752	1/1	0.95	0.10	68,68,68,68	0
56	MG	1A	3391	1/1	0.95	0.17	18,18,18,18	0
56	MG	1A	3034	1/1	0.95	0.25	35,35,35,35	0
56	MG	1A	3118	1/1	0.95	0.18	30,30,30,30	0
56	MG	1A	3396	1/1	0.95	0.15	45,45,45,45	0
56	MG	1N	3005	1/1	0.95	0.20	51,51,51,51	0
56	MG	2A	3555	1/1	0.95	0.12	53,53,53,53	0
56	MG	2A	3035	1/1	0.95	0.12	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	2a	1765	1/1	0.95	0.10	53,53,53,53	0
56	MG	2a	1766	1/1	0.95	0.11	56,56,56,56	0
56	MG	2A	3246	1/1	0.95	0.11	56,56,56,56	0
56	MG	2A	3036	1/1	0.95	0.20	43,43,43,43	0
56	MG	1A	3843	1/1	0.95	0.17	33,33,33,33	0
56	MG	2a	1772	1/1	0.95	0.11	52,52,52,52	0
56	MG	1A	3587	1/1	0.95	0.15	25,25,25,25	0
56	MG	2A	3040	1/1	0.95	0.13	43,43,43,43	0
56	MG	2A	3251	1/1	0.95	0.18	27,27,27,27	0
56	MG	2a	1776	1/1	0.95	0.18	66,66,66,66	0
56	MG	1A	3397	1/1	0.95	0.18	56,56,56,56	0
56	MG	2A	3569	1/1	0.95	0.14	51,51,51,51	0
56	MG	1A	3590	1/1	0.95	0.16	24,24,24,24	0
56	MG	1A	3591	1/1	0.95	0.20	49,49,49,49	0
56	MG	2a	1782	1/1	0.95	0.23	71,71,71,71	0
56	MG	1A	3120	1/1	0.95	0.12	38,38,38,38	0
56	MG	1P	201	1/1	0.95	0.07	50,50,50,50	0
56	MG	1A	3707	1/1	0.95	0.16	54,54,54,54	0
56	MG	1A	3403	1/1	0.95	0.16	52,52,52,52	0
56	MG	1A	3097	1/1	0.95	0.18	16,16,16,16	0
56	MG	1A	3856	1/1	0.95	0.14	29,29,29,29	0
56	MG	1a	1716	1/1	0.95	0.14	62,62,62,62	0
56	MG	1A	3713	1/1	0.95	0.13	36,36,36,36	0
56	MG	1A	3484	1/1	0.95	0.23	30,30,30,30	0
56	MG	1A	3408	1/1	0.95	0.15	43,43,43,43	0
56	MG	1A	3716	1/1	0.95	0.36	59,59,59,59	0
56	MG	2A	3278	1/1	0.95	0.13	31,31,31,31	0
56	MG	1A	3241	1/1	0.95	0.13	51,51,51,51	0
56	MG	2A	3590	1/1	0.95	0.21	41,41,41,41	0
56	MG	2A	3591	1/1	0.95	0.20	45,45,45,45	0
56	MG	1a	1724	1/1	0.95	0.15	52,52,52,52	0
56	MG	2A	3283	1/1	0.95	0.17	51,51,51,51	0
56	MG	2p	3001	1/1	0.95	0.13	52,52,52,52	0
56	MG	2A	3594	1/1	0.95	0.06	48,48,48,48	0
56	MG	2A	3284	1/1	0.95	0.17	49,49,49,49	0
56	MG	1S	3002	1/1	0.95	0.13	53,53,53,53	0
56	MG	2A	3287	1/1	0.95	0.07	31,31,31,31	0
56	MG	2A	3289	1/1	0.95	0.12	60,60,60,60	0
56	MG	1A	3123	1/1	0.95	0.24	43,43,43,43	0
56	MG	1A	3166	1/1	0.95	0.25	44,44,44,44	0
56	MG	1U	201	1/1	0.95	0.19	33,33,33,33	0
56	MG	2A	3607	1/1	0.95	0.17	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	2A	3295	1/1	0.95	0.11	39,39,39,39	0
56	MG	1A	3493	1/1	0.95	0.21	21,21,21,21	0
56	MG	2A	3613	1/1	0.95	0.15	64,64,64,64	0
56	MG	1A	3022	1/1	0.95	0.15	27,27,27,27	0
56	MG	1A	3723	1/1	0.95	0.15	62,62,62,62	0
56	MG	2A	3299	1/1	0.95	0.09	36,36,36,36	0
56	MG	2A	3069	1/1	0.95	0.16	30,30,30,30	0
56	MG	1V	202	1/1	0.95	0.15	59,59,59,59	0
56	MG	2A	3161	1/1	0.96	0.25	49,49,49,49	0
56	MG	1A	3496	1/1	0.96	0.16	28,28,28,28	0
56	MG	2A	3673	1/1	0.96	0.12	33,33,33,33	0
56	MG	1A	3344	1/1	0.96	0.23	48,48,48,48	0
56	MG	1A	3102	1/1	0.96	0.28	44,44,44,44	0
56	MG	1A	3151	1/1	0.96	0.22	34,34,34,34	0
56	MG	2A	3167	1/1	0.96	0.24	39,39,39,39	0
56	MG	1G	202	1/1	0.96	0.15	45,45,45,45	0
56	MG	1f	3002	1/1	0.96	0.15	54,54,54,54	0
56	MG	2B	3005	1/1	0.96	0.20	54,54,54,54	0
56	MG	1l	201	1/1	0.96	0.14	34,34,34,34	0
56	MG	1l	202	1/1	0.96	0.14	52,52,52,52	0
56	MG	1A	3252	1/1	0.96	0.17	41,41,41,41	0
56	MG	2A	3400	1/1	0.96	0.12	49,49,49,49	0
56	MG	1A	3184	1/1	0.96	0.14	34,34,34,34	0
56	MG	2B	3011	1/1	0.96	0.20	55,55,55,55	0
56	MG	1A	3072	1/1	0.96	0.17	40,40,40,40	0
56	MG	1N	3004	1/1	0.96	0.48	56,56,56,56	0
56	MG	2B	3015	1/1	0.96	0.17	48,48,48,48	0
56	MG	1A	3153	1/1	0.96	0.18	31,31,31,31	0
56	MG	1A	3854	1/1	0.96	0.15	33,33,33,33	0
56	MG	2A	3180	1/1	0.96	0.19	39,39,39,39	0
56	MG	1a	1687	1/1	0.96	0.11	55,55,55,55	0
56	MG	1N	3007	1/1	0.96	0.19	25,25,25,25	0
56	MG	1O	201	1/1	0.96	0.15	39,39,39,39	0
56	MG	1x	3002	1/1	0.96	0.15	56,56,56,56	0
56	MG	1A	3506	1/1	0.96	0.14	62,62,62,62	0
56	MG	1A	3727	1/1	0.96	0.16	45,45,45,45	0
56	MG	1A	3728	1/1	0.96	0.20	50,50,50,50	0
56	MG	2F	302	1/1	0.96	0.24	50,50,50,50	0
56	MG	2A	3420	1/1	0.96	0.10	43,43,43,43	0
56	MG	1A	3295	1/1	0.96	0.15	43,43,43,43	0
56	MG	2A	3422	1/1	0.96	0.12	43,43,43,43	0
56	MG	2A	3423	1/1	0.96	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	1x	3007	1/1	0.96	0.28	51,51,51,51	0
56	MG	2A	3193	1/1	0.96	0.11	40,40,40,40	0
56	MG	1a	1694	1/1	0.96	0.20	66,66,66,66	0
56	MG	2Q	203	1/1	0.96	0.16	37,37,37,37	0
56	MG	1A	3155	1/1	0.96	0.14	48,48,48,48	0
56	MG	2R	201	1/1	0.96	0.15	48,48,48,48	0
56	MG	2A	3430	1/1	0.96	0.14	56,56,56,56	0
56	MG	2U	203	1/1	0.96	0.24	42,42,42,42	0
56	MG	2A	3196	1/1	0.96	0.10	35,35,35,35	0
56	MG	1A	3731	1/1	0.96	0.15	58,58,58,58	0
56	MG	2A	3436	1/1	0.96	0.17	39,39,39,39	0
56	MG	1y	102	1/1	0.96	0.12	63,63,63,63	0
56	MG	2A	3439	1/1	0.96	0.12	36,36,36,36	0
56	MG	2A	3199	1/1	0.96	0.23	43,43,43,43	0
56	MG	1A	3509	1/1	0.96	0.13	31,31,31,31	0
56	MG	1P	203	1/1	0.96	0.29	27,27,27,27	0
56	MG	2A	3443	1/1	0.96	0.14	36,36,36,36	0
56	MG	2A	3444	1/1	0.96	0.21	50,50,50,50	0
56	MG	2A	3445	1/1	0.96	0.08	39,39,39,39	0
56	MG	1A	3733	1/1	0.96	0.15	25,25,25,25	0
56	MG	2A	3004	1/1	0.96	0.14	36,36,36,36	0
56	MG	2A	3205	1/1	0.96	0.29	53,53,53,53	0
56	MG	2A	3451	1/1	0.96	0.32	36,36,36,36	0
56	MG	1A	3297	1/1	0.96	0.16	19,19,19,19	0
56	MG	2A	3453	1/1	0.96	0.10	37,37,37,37	0
56	MG	2a	1610	1/1	0.96	0.33	52,52,52,52	0
56	MG	1A	3735	1/1	0.96	0.19	25,25,25,25	0
56	MG	2A	3459	1/1	0.96	0.15	49,49,49,49	0
56	MG	1A	3871	1/1	0.96	0.16	18,18,18,18	0
56	MG	2A	3008	1/1	0.96	0.20	39,39,39,39	0
56	MG	2A	3463	1/1	0.96	0.09	45,45,45,45	0
56	MG	2A	3211	1/1	0.96	0.13	43,43,43,43	0
56	MG	1A	3736	1/1	0.96	0.23	38,38,38,38	0
56	MG	1A	3620	1/1	0.96	0.15	32,32,32,32	0
56	MG	2a	1620	1/1	0.96	0.09	58,58,58,58	0
56	MG	1A	3622	1/1	0.96	0.12	52,52,52,52	0
56	MG	1A	3740	1/1	0.96	0.06	39,39,39,39	0
56	MG	1A	3511	1/1	0.96	0.15	49,49,49,49	0
56	MG	2A	3017	1/1	0.96	0.14	26,26,26,26	0
56	MG	1A	3422	1/1	0.96	0.14	45,45,45,45	0
56	MG	1A	3299	1/1	0.96	0.25	40,40,40,40	0
56	MG	2A	3221	1/1	0.96	0.20	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	1A	3744	1/1	0.96	0.15	50,50,50,50	0
56	MG	1A	3357	1/1	0.96	0.28	52,52,52,52	0
56	MG	2a	1632	1/1	0.96	0.13	59,59,59,59	0
56	MG	1A	3516	1/1	0.96	0.16	25,25,25,25	0
56	MG	1U	205	1/1	0.96	0.21	29,29,29,29	0
56	MG	1A	3038	1/1	0.96	0.21	36,36,36,36	0
56	MG	1A	3008	1/1	0.96	0.17	26,26,26,26	0
56	MG	2a	1638	1/1	0.96	0.10	50,50,50,50	0
56	MG	1A	3361	1/1	0.96	0.11	33,33,33,33	0
56	MG	2a	1640	1/1	0.96	0.11	56,56,56,56	0
56	MG	2A	3033	1/1	0.96	0.14	29,29,29,29	0
56	MG	2A	3034	1/1	0.96	0.15	40,40,40,40	0
56	MG	1A	3106	1/1	0.96	0.18	37,37,37,37	0
56	MG	1A	3430	1/1	0.96	0.10	21,21,21,21	0
56	MG	1W	3005	1/1	0.96	0.09	30,30,30,30	0
56	MG	1A	3304	1/1	0.96	0.12	48,48,48,48	0
56	MG	1X	3001	1/1	0.96	0.27	33,33,33,33	0
56	MG	1A	3364	1/1	0.96	0.16	55,55,55,55	0
56	MG	1A	3040	1/1	0.96	0.12	32,32,32,32	0
56	MG	1Y	502	1/1	0.96	0.28	50,50,50,50	0
56	MG	2A	3239	1/1	0.96	0.10	43,43,43,43	0
56	MG	1A	3527	1/1	0.96	0.11	41,41,41,41	0
56	MG	1A	3306	1/1	0.96	0.30	55,55,55,55	0
56	MG	1A	3263	1/1	0.96	0.23	41,41,41,41	0
56	MG	1a	1740	1/1	0.96	0.11	45,45,45,45	0
56	MG	2A	3500	1/1	0.96	0.11	38,38,38,38	0
56	MG	1A	3013	1/1	0.96	0.26	24,24,24,24	0
56	MG	1A	3109	1/1	0.96	0.55	34,34,34,34	0
56	MG	1A	3311	1/1	0.96	0.26	50,50,50,50	0
56	MG	2a	1662	1/1	0.96	0.21	42,42,42,42	0
56	MG	2a	1663	1/1	0.96	0.24	62,62,62,62	0
56	MG	1A	3077	1/1	0.96	0.15	39,39,39,39	0
56	MG	2A	3507	1/1	0.96	0.16	19,19,19,19	0
56	MG	2A	3054	1/1	0.96	0.09	41,41,41,41	0
56	MG	1a	1745	1/1	0.96	0.13	43,43,43,43	0
56	MG	1A	3444	1/1	0.96	0.10	37,37,37,37	0
56	MG	1A	3906	1/1	0.96	0.15	42,42,42,42	0
56	MG	1A	3767	1/1	0.96	0.14	39,39,39,39	0
56	MG	13	101	1/1	0.96	0.11	50,50,50,50	0
56	MG	2A	3515	1/1	0.96	0.12	35,35,35,35	0
56	MG	1A	3908	1/1	0.96	0.42	38,38,38,38	0
56	MG	1A	3445	1/1	0.96	0.11	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	15	102	1/1	0.96	0.10	37,37,37,37	0
56	MG	1A	3541	1/1	0.96	0.08	42,42,42,42	0
56	MG	2A	3262	1/1	0.96	0.14	41,41,41,41	0
56	MG	1a	1754	1/1	0.96	0.10	45,45,45,45	0
56	MG	2A	3264	1/1	0.96	0.25	40,40,40,40	0
56	MG	1A	3446	1/1	0.96	0.03	48,48,48,48	0
56	MG	2A	3268	1/1	0.96	0.12	37,37,37,37	0
56	MG	1A	3134	1/1	0.96	0.12	35,35,35,35	0
56	MG	1a	1757	1/1	0.96	0.14	39,39,39,39	0
56	MG	18	101	1/1	0.96	0.31	45,45,45,45	0
56	MG	18	102	1/1	0.96	0.17	33,33,33,33	0
56	MG	2A	3273	1/1	0.96	0.12	35,35,35,35	0
56	MG	1A	3448	1/1	0.96	0.11	57,57,57,57	0
56	MG	1A	3653	1/1	0.96	0.13	47,47,47,47	0
56	MG	1A	3657	1/1	0.96	0.09	29,29,29,29	0
56	MG	1A	3043	1/1	0.96	0.12	27,27,27,27	0
56	MG	1A	3776	1/1	0.96	0.21	45,45,45,45	0
56	MG	2a	1694	1/1	0.96	0.21	62,62,62,62	0
56	MG	1A	3375	1/1	0.96	0.17	32,32,32,32	0
56	MG	1A	3550	1/1	0.96	0.16	40,40,40,40	0
56	MG	2a	1697	1/1	0.96	0.14	37,37,37,37	0
56	MG	1A	3453	1/1	0.96	0.10	31,31,31,31	0
56	MG	2a	1699	1/1	0.96	0.12	38,38,38,38	0
56	MG	2A	3546	1/1	0.96	0.14	33,33,33,33	0
56	MG	2A	3080	1/1	0.96	0.17	50,50,50,50	0
56	MG	2A	3288	1/1	0.96	0.10	44,44,44,44	0
56	MG	1a	1772	1/1	0.96	0.10	60,60,60,60	0
56	MG	1A	3664	1/1	0.96	0.16	39,39,39,39	0
56	MG	1A	3136	1/1	0.96	0.11	39,39,39,39	0
56	MG	1a	1775	1/1	0.96	0.07	52,52,52,52	0
56	MG	1A	3377	1/1	0.96	0.17	36,36,36,36	0
56	MG	1A	3937	1/1	0.96	0.25	39,39,39,39	0
56	MG	1A	3378	1/1	0.96	0.21	43,43,43,43	0
56	MG	1A	3201	1/1	0.96	0.20	39,39,39,39	0
56	MG	1a	1781	1/1	0.96	0.17	63,63,63,63	0
56	MG	1A	3941	1/1	0.96	0.10	43,43,43,43	0
56	MG	1A	3234	1/1	0.96	0.31	34,34,34,34	0
56	MG	2A	3563	1/1	0.96	0.09	36,36,36,36	0
56	MG	2a	1719	1/1	0.96	0.17	44,44,44,44	0
56	MG	1A	3789	1/1	0.96	0.09	33,33,33,33	0
56	MG	1A	3065	1/1	0.96	0.17	14,14,14,14	0
56	MG	1A	3382	1/1	0.96	0.18	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	3561	1/1	0.96	0.16	54,54,54,54	0
56	MG	1A	3324	1/1	0.96	0.12	43,43,43,43	0
56	MG	2A	3571	1/1	0.96	0.14	47,47,47,47	0
56	MG	1A	3204	1/1	0.96	0.15	24,24,24,24	0
56	MG	1A	3205	1/1	0.96	0.15	33,33,33,33	0
56	MG	2A	3310	1/1	0.96	0.21	34,34,34,34	0
56	MG	1A	3386	1/1	0.96	0.16	42,42,42,42	0
56	MG	1A	3680	1/1	0.96	0.33	36,36,36,36	0
56	MG	2A	3314	1/1	0.96	0.15	40,40,40,40	0
56	MG	1A	3959	1/1	0.96	0.38	53,53,53,53	0
56	MG	2A	3106	1/1	0.96	0.13	28,28,28,28	0
56	MG	2a	1735	1/1	0.96	0.22	42,42,42,42	0
56	MG	2A	3318	1/1	0.96	0.19	38,38,38,38	0
56	MG	1A	3470	1/1	0.96	0.17	27,27,27,27	0
56	MG	1A	3387	1/1	0.96	0.13	38,38,38,38	0
56	MG	1A	3684	1/1	0.96	0.16	29,29,29,29	0
56	MG	1A	3096	1/1	0.96	0.15	22,22,22,22	0
56	MG	2a	1741	1/1	0.96	0.25	48,48,48,48	0
56	MG	1A	3808	1/1	0.96	0.23	41,41,41,41	0
56	MG	2A	3589	1/1	0.96	0.08	41,41,41,41	0
56	MG	2A	3325	1/1	0.96	0.09	25,25,25,25	0
56	MG	2A	3327	1/1	0.96	0.14	33,33,33,33	0
56	MG	1A	3571	1/1	0.96	0.19	39,39,39,39	0
56	MG	2a	1749	1/1	0.96	0.19	58,58,58,58	0
56	MG	2a	1750	1/1	0.96	0.17	72,72,72,72	0
56	MG	1A	3572	1/1	0.96	0.13	33,33,33,33	0
56	MG	1A	3574	1/1	0.96	0.16	47,47,47,47	0
56	MG	2A	3596	1/1	0.96	0.10	42,42,42,42	0
56	MG	2A	3597	1/1	0.96	0.16	46,46,46,46	0
56	MG	1A	3690	1/1	0.96	0.11	48,48,48,48	0
56	MG	2a	1758	1/1	0.96	0.16	46,46,46,46	0
56	MG	1A	3002	1/1	0.96	0.31	61,61,61,61	0
56	MG	2A	3337	1/1	0.96	0.16	42,42,42,42	0
56	MG	2a	1761	1/1	0.96	0.09	82,82,82,82	0
56	MG	2A	3338	1/1	0.96	0.10	42,42,42,42	0
56	MG	1A	3814	1/1	0.96	0.19	16,16,16,16	0
56	MG	1A	3330	1/1	0.96	0.21	42,42,42,42	0
56	MG	1A	3048	1/1	0.96	0.23	32,32,32,32	0
56	MG	2A	3606	1/1	0.96	0.06	51,51,51,51	0
56	MG	2a	1768	1/1	0.96	0.13	54,54,54,54	0
56	MG	1A	3579	1/1	0.96	0.19	21,21,21,21	0
56	MG	2a	1770	1/1	0.96	0.20	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	1A	3478	1/1	0.96	0.16	20,20,20,20	0
56	MG	1A	3069	1/1	0.96	0.13	27,27,27,27	0
56	MG	2A	3612	1/1	0.96	0.13	57,57,57,57	0
56	MG	1A	3037	1/1	0.96	0.09	38,38,38,38	0
56	MG	2A	3349	1/1	0.96	0.18	18,18,18,18	0
56	MG	2A	3350	1/1	0.96	0.12	38,38,38,38	0
56	MG	1A	3179	1/1	0.96	0.22	31,31,31,31	0
56	MG	2A	3352	1/1	0.96	0.20	55,55,55,55	0
56	MG	1A	3245	1/1	0.96	0.20	29,29,29,29	0
56	MG	2A	3620	1/1	0.96	0.14	39,39,39,39	0
56	MG	2A	3354	1/1	0.96	0.18	43,43,43,43	0
56	MG	1a	1817	1/1	0.96	0.19	48,48,48,48	0
56	MG	1B	3017	1/1	0.96	0.12	44,44,44,44	0
56	MG	2A	3358	1/1	0.96	0.10	52,52,52,52	0
56	MG	2a	1787	1/1	0.96	0.23	51,51,51,51	0
56	MG	2A	3129	1/1	0.96	0.22	41,41,41,41	0
56	MG	1A	3399	1/1	0.96	0.16	42,42,42,42	0
56	MG	1B	3022	1/1	0.96	0.09	53,53,53,53	0
56	MG	1A	3702	1/1	0.96	0.14	45,45,45,45	0
56	MG	2A	3364	1/1	0.96	0.14	31,31,31,31	0
56	MG	1A	3283	1/1	0.96	0.16	37,37,37,37	0
56	MG	1A	3402	1/1	0.96	0.15	38,38,38,38	0
56	MG	1a	1825	1/1	0.96	0.11	46,46,46,46	0
56	MG	2A	3635	1/1	0.96	0.11	38,38,38,38	0
56	MG	1A	3338	1/1	0.96	0.08	36,36,36,36	0
56	MG	2f	3001	1/1	0.96	0.13	39,39,39,39	0
56	MG	1A	3489	1/1	0.96	0.17	40,40,40,40	0
56	MG	1B	3029	1/1	0.96	0.12	28,28,28,28	0
56	MG	1A	3406	1/1	0.96	0.18	23,23,23,23	0
56	MG	2l	201	1/1	0.96	0.09	61,61,61,61	0
56	MG	1A	3834	1/1	0.96	0.37	46,46,46,46	0
56	MG	2A	3642	1/1	0.96	0.17	32,32,32,32	0
56	MG	1A	3708	1/1	0.96	0.20	47,47,47,47	0
56	MG	1A	3491	1/1	0.96	0.09	53,53,53,53	0
56	MG	2A	3148	1/1	0.96	0.21	43,43,43,43	0
56	MG	1A	3119	1/1	0.96	0.43	36,36,36,36	0
56	MG	1A	3247	1/1	0.96	0.24	27,27,27,27	0
56	MG	1E	305	1/1	0.96	0.20	37,37,37,37	0
56	MG	2A	3152	1/1	0.96	0.12	32,32,32,32	0
56	MG	2A	3654	1/1	0.96	0.13	34,34,34,34	0
56	MG	1F	301	1/1	0.96	0.14	51,51,51,51	0
56	MG	2A	3656	1/1	0.96	0.46	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	2A	3158	1/1	0.96	0.14	49,49,49,49	0
58	HGR	2A	3652	36/36	0.96	0.24	21,36,48,50	0
56	MG	1A	3071	1/1	0.96	0.16	47,47,47,47	0
56	MG	2A	3659	1/1	0.96	0.58	43,43,43,43	0
56	MG	1A	3410	1/1	0.96	0.21	42,42,42,42	0
56	MG	2A	3387	1/1	0.96	0.28	50,50,50,50	0
56	MG	2A	3662	1/1	0.96	0.27	29,29,29,29	0
56	MG	2A	3665	1/1	0.96	0.09	57,57,57,57	0
56	MG	1A	3936	1/1	0.97	0.28	29,29,29,29	0
56	MG	1a	1698	1/1	0.97	0.18	51,51,51,51	0
56	MG	2A	3502	1/1	0.97	0.05	35,35,35,35	0
56	MG	2A	3301	1/1	0.97	0.09	35,35,35,35	0
56	MG	1A	3078	1/1	0.97	0.25	38,38,38,38	0
56	MG	2a	1601	1/1	0.97	0.25	45,45,45,45	0
56	MG	1A	3661	1/1	0.97	0.20	45,45,45,45	0
56	MG	1A	3737	1/1	0.97	0.19	50,50,50,50	0
56	MG	2A	3508	1/1	0.97	0.09	38,38,38,38	0
56	MG	1X	3003	1/1	0.97	0.23	32,32,32,32	0
56	MG	1a	1703	1/1	0.97	0.15	50,50,50,50	0
56	MG	1A	3940	1/1	0.97	0.51	33,33,33,33	0
56	MG	2A	3132	1/1	0.97	0.13	44,44,44,44	0
56	MG	1A	3825	1/1	0.97	0.17	47,47,47,47	0
56	MG	1A	3089	1/1	0.97	0.15	40,40,40,40	0
56	MG	1t	3001	1/1	0.97	0.15	47,47,47,47	0
56	MG	2A	3516	1/1	0.97	0.15	46,46,46,46	0
56	MG	2A	3517	1/1	0.97	0.11	54,54,54,54	0
56	MG	2a	1615	1/1	0.97	0.18	63,63,63,63	0
56	MG	1A	3128	1/1	0.97	0.27	49,49,49,49	0
56	MG	2A	3313	1/1	0.97	0.11	37,37,37,37	0
56	MG	1a	1708	1/1	0.97	0.21	34,34,34,34	0
56	MG	1A	3255	1/1	0.97	0.21	50,50,50,50	0
56	MG	2A	3139	1/1	0.97	0.22	38,38,38,38	0
56	MG	1A	3312	1/1	0.97	0.22	41,41,41,41	0
56	MG	1A	3079	1/1	0.97	0.35	30,30,30,30	0
56	MG	1a	1712	1/1	0.97	0.20	49,49,49,49	0
56	MG	2A	3526	1/1	0.97	0.13	49,49,49,49	0
56	MG	2A	3143	1/1	0.97	0.13	47,47,47,47	0
56	MG	2A	3322	1/1	0.97	0.13	49,49,49,49	0
56	MG	2a	1627	1/1	0.97	0.08	46,46,46,46	0
56	MG	1a	1714	1/1	0.97	0.23	42,42,42,42	0
56	MG	1A	3530	1/1	0.97	0.13	14,14,14,14	0
56	MG	1A	3951	1/1	0.97	0.22	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	3045	1/1	0.97	0.19	19,19,19,19	0
56	MG	1l	102	1/1	0.97	0.14	38,38,38,38	0
56	MG	1A	3835	1/1	0.97	0.33	30,30,30,30	0
56	MG	1A	3954	1/1	0.97	0.19	28,28,28,28	0
56	MG	2a	1636	1/1	0.97	0.08	60,60,60,60	0
56	MG	2A	3536	1/1	0.97	0.11	46,46,46,46	0
56	MG	1a	1722	1/1	0.97	0.13	50,50,50,50	0
56	MG	1A	3315	1/1	0.97	0.36	37,37,37,37	0
56	MG	2A	3539	1/1	0.97	0.10	51,51,51,51	0
56	MG	1A	3957	1/1	0.97	0.32	37,37,37,37	0
56	MG	1A	3599	1/1	0.97	0.21	28,28,28,28	0
56	MG	2A	3544	1/1	0.97	0.10	53,53,53,53	0
56	MG	2a	1644	1/1	0.97	0.10	66,66,66,66	0
56	MG	1y	101	1/1	0.97	0.29	38,38,38,38	0
56	MG	1A	3189	1/1	0.97	0.15	32,32,32,32	0
56	MG	2A	3163	1/1	0.97	0.17	32,32,32,32	0
56	MG	15	103	1/1	0.97	0.09	53,53,53,53	0
56	MG	2A	3344	1/1	0.97	0.10	30,30,30,30	0
56	MG	1A	3355	1/1	0.97	0.22	46,46,46,46	0
56	MG	2A	3346	1/1	0.97	0.07	36,36,36,36	0
56	MG	2A	3552	1/1	0.97	0.10	57,57,57,57	0
56	MG	1A	3840	1/1	0.97	0.26	36,36,36,36	0
56	MG	1a	1731	1/1	0.97	0.15	61,61,61,61	0
56	MG	1A	3047	1/1	0.97	0.16	35,35,35,35	0
56	MG	1A	3538	1/1	0.97	0.14	40,40,40,40	0
56	MG	1A	3539	1/1	0.97	0.25	51,51,51,51	0
56	MG	1A	3752	1/1	0.97	0.10	37,37,37,37	0
56	MG	1a	1737	1/1	0.97	0.14	33,33,33,33	0
56	MG	2A	3010	1/1	0.97	0.13	30,30,30,30	0
56	MG	1A	3753	1/1	0.97	0.05	49,49,49,49	0
56	MG	1A	3754	1/1	0.97	0.11	53,53,53,53	0
56	MG	2A	3565	1/1	0.97	0.15	50,50,50,50	0
56	MG	1A	3678	1/1	0.97	0.15	36,36,36,36	0
56	MG	2A	3178	1/1	0.97	0.20	43,43,43,43	0
56	MG	2A	3568	1/1	0.97	0.11	54,54,54,54	0
56	MG	1A	3485	1/1	0.97	0.23	38,38,38,38	0
56	MG	2A	3015	1/1	0.97	0.24	36,36,36,36	0
56	MG	2A	3016	1/1	0.97	0.15	41,41,41,41	0
56	MG	1A	3319	1/1	0.97	0.42	28,28,28,28	0
56	MG	1A	3358	1/1	0.97	0.14	33,33,33,33	0
56	MG	2A	3185	1/1	0.97	0.25	55,55,55,55	0
56	MG	2A	3020	1/1	0.97	0.08	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	2A	3022	1/1	0.97	0.34	43,43,43,43	0
56	MG	2a	1676	1/1	0.97	0.21	40,40,40,40	0
56	MG	1A	3682	1/1	0.97	0.14	50,50,50,50	0
56	MG	1A	3019	1/1	0.97	0.13	27,27,27,27	0
56	MG	1A	3041	1/1	0.97	0.16	35,35,35,35	0
56	MG	2A	3581	1/1	0.97	0.14	66,66,66,66	0
56	MG	1A	3858	1/1	0.97	0.13	36,36,36,36	0
56	MG	1a	1610	1/1	0.97	0.10	22,22,22,22	0
56	MG	1A	3288	1/1	0.97	0.18	36,36,36,36	0
56	MG	1A	3763	1/1	0.97	0.19	39,39,39,39	0
56	MG	2A	3030	1/1	0.97	0.11	28,28,28,28	0
56	MG	2A	3031	1/1	0.97	0.07	24,24,24,24	0
56	MG	1A	3442	1/1	0.97	0.16	36,36,36,36	0
56	MG	1A	3864	1/1	0.97	0.09	38,38,38,38	0
56	MG	1B	3018	1/1	0.97	0.20	41,41,41,41	0
56	MG	1B	3019	1/1	0.97	0.14	22,22,22,22	0
56	MG	2A	3384	1/1	0.97	0.10	39,39,39,39	0
56	MG	2A	3202	1/1	0.97	0.19	44,44,44,44	0
56	MG	1B	3020	1/1	0.97	0.15	48,48,48,48	0
56	MG	1A	3549	1/1	0.97	0.17	41,41,41,41	0
56	MG	2A	3038	1/1	0.97	0.23	48,48,48,48	0
56	MG	1A	3688	1/1	0.97	0.15	41,41,41,41	0
56	MG	2A	3600	1/1	0.97	0.10	42,42,42,42	0
56	MG	1A	3867	1/1	0.97	0.09	31,31,31,31	0
56	MG	1a	1622	1/1	0.97	0.13	49,49,49,49	0
56	MG	1A	3614	1/1	0.97	0.16	42,42,42,42	0
56	MG	1A	3615	1/1	0.97	0.12	45,45,45,45	0
56	MG	1a	1625	1/1	0.97	0.22	53,53,53,53	0
56	MG	1A	3215	1/1	0.97	0.19	56,56,56,56	0
56	MG	1a	1765	1/1	0.97	0.18	69,69,69,69	0
56	MG	2A	3397	1/1	0.97	0.14	36,36,36,36	0
56	MG	2A	3609	1/1	0.97	0.16	36,36,36,36	0
56	MG	2a	1708	1/1	0.97	0.07	52,52,52,52	0
56	MG	1A	3552	1/1	0.97	0.16	22,22,22,22	0
56	MG	2a	1710	1/1	0.97	0.09	61,61,61,61	0
56	MG	2A	3611	1/1	0.97	0.08	60,60,60,60	0
56	MG	2a	1712	1/1	0.97	0.21	58,58,58,58	0
56	MG	2a	1713	1/1	0.97	0.11	49,49,49,49	0
56	MG	1A	3216	1/1	0.97	0.41	36,36,36,36	0
56	MG	1A	3027	1/1	0.97	0.28	33,33,33,33	0
56	MG	2A	3614	1/1	0.97	0.10	54,54,54,54	0
56	MG	1A	3405	1/1	0.97	0.16	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3219	1/1	0.97	0.24	45,45,45,45	0
56	MG	2A	3403	1/1	0.97	0.17	37,37,37,37	0
56	MG	1D	303	1/1	0.97	0.30	25,25,25,25	0
56	MG	1A	3240	1/1	0.97	0.19	40,40,40,40	0
56	MG	1D	305	1/1	0.97	0.23	31,31,31,31	0
56	MG	1A	3174	1/1	0.97	0.22	34,34,34,34	0
56	MG	1A	3877	1/1	0.97	0.11	49,49,49,49	0
56	MG	2A	3409	1/1	0.97	0.23	42,42,42,42	0
56	MG	1A	3878	1/1	0.97	0.13	40,40,40,40	0
56	MG	1A	3499	1/1	0.97	0.12	34,34,34,34	0
56	MG	1E	306	1/1	0.97	0.16	56,56,56,56	0
56	MG	2A	3062	1/1	0.97	0.16	42,42,42,42	0
56	MG	1A	3450	1/1	0.97	0.13	42,42,42,42	0
56	MG	2A	3629	1/1	0.97	0.07	56,56,56,56	0
56	MG	2A	3630	1/1	0.97	0.12	41,41,41,41	0
56	MG	1A	3451	1/1	0.97	0.15	40,40,40,40	0
56	MG	1A	3294	1/1	0.97	0.17	32,32,32,32	0
56	MG	1A	3268	1/1	0.97	0.23	33,33,33,33	0
56	MG	1a	1785	1/1	0.97	0.20	41,41,41,41	0
56	MG	1a	1786	1/1	0.97	0.11	56,56,56,56	0
56	MG	1A	3195	1/1	0.97	0.10	39,39,39,39	0
56	MG	1A	3456	1/1	0.97	0.18	28,28,28,28	0
56	MG	1A	3632	1/1	0.97	0.17	57,57,57,57	0
56	MG	2A	3427	1/1	0.97	0.14	42,42,42,42	0
56	MG	2A	3428	1/1	0.97	0.14	27,27,27,27	0
56	MG	2a	1744	1/1	0.97	0.11	47,47,47,47	0
56	MG	1A	3887	1/1	0.97	0.08	49,49,49,49	0
56	MG	2a	1746	1/1	0.97	0.11	59,59,59,59	0
56	MG	1a	1648	1/1	0.97	0.24	43,43,43,43	0
56	MG	2A	3433	1/1	0.97	0.16	41,41,41,41	0
56	MG	1A	3785	1/1	0.97	0.15	37,37,37,37	0
56	MG	1A	3565	1/1	0.97	0.14	28,28,28,28	0
56	MG	2A	3647	1/1	0.97	0.19	41,41,41,41	0
56	MG	1N	3001	1/1	0.97	0.42	38,38,38,38	0
56	MG	2A	3650	1/1	0.97	0.12	37,37,37,37	0
56	MG	2a	1755	1/1	0.97	0.12	61,61,61,61	0
56	MG	1A	3067	1/1	0.97	0.16	18,18,18,18	0
56	MG	1A	3154	1/1	0.97	0.35	36,36,36,36	0
56	MG	1A	3636	1/1	0.97	0.17	53,53,53,53	0
56	MG	1A	3711	1/1	0.97	0.17	41,41,41,41	0
56	MG	1A	3712	1/1	0.97	0.22	50,50,50,50	0
56	MG	1A	3897	1/1	0.97	0.49	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1a	1659	1/1	0.97	0.23	55,55,55,55	0
56	MG	1A	3413	1/1	0.97	0.13	30,30,30,30	0
56	MG	1A	3300	1/1	0.97	0.21	31,31,31,31	0
56	MG	1a	1663	1/1	0.97	0.10	59,59,59,59	0
56	MG	2A	3253	1/1	0.97	0.11	47,47,47,47	0
56	MG	2A	3664	1/1	0.97	0.51	46,46,46,46	0
56	MG	2A	3449	1/1	0.97	0.12	42,42,42,42	0
56	MG	2A	3666	1/1	0.97	0.18	48,48,48,48	0
56	MG	2A	3450	1/1	0.97	0.12	24,24,24,24	0
56	MG	1A	3373	1/1	0.97	0.20	53,53,53,53	0
56	MG	2A	3670	1/1	0.97	0.16	57,57,57,57	0
56	MG	2A	3671	1/1	0.97	0.05	51,51,51,51	0
56	MG	1A	3336	1/1	0.97	0.17	40,40,40,40	0
56	MG	2A	3257	1/1	0.97	0.13	47,47,47,47	0
56	MG	2A	3455	1/1	0.97	0.20	44,44,44,44	0
56	MG	2A	3089	1/1	0.97	0.10	27,27,27,27	0
56	MG	2A	3457	1/1	0.97	0.09	48,48,48,48	0
56	MG	2A	3458	1/1	0.97	0.17	57,57,57,57	0
56	MG	1A	3001	1/1	0.97	0.10	33,33,33,33	0
56	MG	1A	3035	1/1	0.97	0.33	32,32,32,32	0
56	MG	1A	3905	1/1	0.97	0.12	35,35,35,35	0
56	MG	1A	3802	1/1	0.97	0.10	60,60,60,60	0
56	MG	1A	3576	1/1	0.97	0.10	41,41,41,41	0
56	MG	1A	3158	1/1	0.97	0.14	49,49,49,49	0
56	MG	1A	3909	1/1	0.97	0.13	36,36,36,36	0
56	MG	1Q	203	1/1	0.97	0.22	33,33,33,33	0
56	MG	1Q	204	1/1	0.97	0.12	55,55,55,55	0
56	MG	1A	3721	1/1	0.97	0.10	50,50,50,50	0
56	MG	1A	3807	1/1	0.97	0.21	49,49,49,49	0
56	MG	1A	3110	1/1	0.97	0.19	29,29,29,29	0
56	MG	2A	3472	1/1	0.97	0.15	55,55,55,55	0
56	MG	1R	202	1/1	0.97	0.22	36,36,36,36	0
56	MG	2A	3275	1/1	0.97	0.13	46,46,46,46	0
56	MG	2e	3001	1/1	0.97	0.10	53,53,53,53	0
56	MG	1a	1822	1/1	0.97	0.14	62,62,62,62	0
56	MG	2A	3476	1/1	0.97	0.13	47,47,47,47	0
56	MG	2A	3477	1/1	0.97	0.16	44,44,44,44	0
56	MG	2j	8001	1/1	0.97	0.13	69,69,69,69	0
56	MG	1A	3469	1/1	0.97	0.16	33,33,33,33	0
56	MG	2A	3279	1/1	0.97	0.13	43,43,43,43	0
56	MG	2A	3280	1/1	0.97	0.21	42,42,42,42	0
56	MG	1A	3724	1/1	0.97	0.18	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3580	1/1	0.97	0.11	32,32,32,32	0
56	MG	2q	3002	1/1	0.97	0.18	63,63,63,63	0
56	MG	1A	3520	1/1	0.97	0.11	47,47,47,47	0
56	MG	1T	202	1/1	0.97	0.09	46,46,46,46	0
56	MG	1A	3161	1/1	0.97	0.20	41,41,41,41	0
56	MG	2A	3286	1/1	0.97	0.18	55,55,55,55	0
56	MG	1A	3583	1/1	0.97	0.18	57,57,57,57	0
56	MG	1A	3926	1/1	0.97	0.27	29,29,29,29	0
56	MG	1A	3471	1/1	0.97	0.13	26,26,26,26	0
56	MG	2A	3290	1/1	0.97	0.12	40,40,40,40	0
56	MG	1A	3654	1/1	0.97	0.10	40,40,40,40	0
56	MG	2T	3001	1/1	0.97	0.14	50,50,50,50	0
58	HGR	1A	3915	36/36	0.97	0.23	15,30,37,44	0
56	MG	1a	1834	1/1	0.97	0.21	44,44,44,44	0
56	MG	1A	3655	1/1	0.97	0.17	52,52,52,52	0
59	ZN	2Y	501	1/1	0.97	0.14	83,83,83,83	0
56	MG	2A	3294	1/1	0.97	0.13	38,38,38,38	0
56	MG	1A	3656	1/1	0.97	0.12	48,48,48,48	0
56	MG	1A	3933	1/1	0.97	0.17	28,28,28,28	0
56	MG	1A	3140	1/1	0.97	0.22	41,41,41,41	0
56	MG	1A	3588	1/1	0.97	0.29	39,39,39,39	0
56	MG	1A	3122	1/1	0.98	0.29	40,40,40,40	0
56	MG	1A	3650	1/1	0.98	0.14	31,31,31,31	0
56	MG	2A	3095	1/1	0.98	0.16	47,47,47,47	0
56	MG	1A	3160	1/1	0.98	0.13	26,26,26,26	0
56	MG	1A	3820	1/1	0.98	0.21	45,45,45,45	0
56	MG	2A	3098	1/1	0.98	0.07	37,37,37,37	0
56	MG	1A	3652	1/1	0.98	0.25	25,25,25,25	0
56	MG	2A	3638	1/1	0.98	0.10	55,55,55,55	0
56	MG	1W	3003	1/1	0.98	0.14	25,25,25,25	0
56	MG	1A	3309	1/1	0.98	0.19	36,36,36,36	0
56	MG	1a	1658	1/1	0.98	0.30	51,51,51,51	0
56	MG	1A	3890	1/1	0.98	0.16	38,38,38,38	0
56	MG	2A	3104	1/1	0.98	0.38	46,46,46,46	0
56	MG	1A	3058	1/1	0.98	0.21	44,44,44,44	0
56	MG	2A	3356	1/1	0.98	0.07	29,29,29,29	0
56	MG	1A	3513	1/1	0.98	0.23	29,29,29,29	0
56	MG	1a	1662	1/1	0.98	0.22	51,51,51,51	0
56	MG	1A	3046	1/1	0.98	0.17	29,29,29,29	0
56	MG	2A	3649	1/1	0.98	0.19	30,30,30,30	0
56	MG	1a	1762	1/1	0.98	0.14	42,42,42,42	0
56	MG	1A	3443	1/1	0.98	0.19	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3362	1/1	0.98	0.19	44,44,44,44	0
56	MG	1A	3658	1/1	0.98	0.33	35,35,35,35	0
56	MG	2A	3505	1/1	0.98	0.20	48,48,48,48	0
56	MG	1a	1666	1/1	0.98	0.17	36,36,36,36	0
56	MG	1A	3030	1/1	0.98	0.46	33,33,33,33	0
56	MG	1B	3015	1/1	0.98	0.15	31,31,31,31	0
56	MG	1A	3517	1/1	0.98	0.11	9,9,9,9	0
56	MG	2a	1692	1/1	0.98	0.14	54,54,54,54	0
56	MG	1A	3208	1/1	0.98	0.24	24,24,24,24	0
56	MG	1A	3258	1/1	0.98	0.17	32,32,32,32	0
56	MG	2A	3118	1/1	0.98	0.11	37,37,37,37	0
56	MG	2A	3663	1/1	0.98	0.28	42,42,42,42	0
56	MG	1A	3901	1/1	0.98	0.16	46,46,46,46	0
56	MG	2A	3372	1/1	0.98	0.22	41,41,41,41	0
56	MG	1A	3832	1/1	0.98	0.10	57,57,57,57	0
56	MG	10	102	1/1	0.98	0.20	62,62,62,62	0
56	MG	2A	3668	1/1	0.98	0.77	48,48,48,48	0
56	MG	1a	1675	1/1	0.98	0.08	40,40,40,40	0
56	MG	1A	3833	1/1	0.98	0.13	54,54,54,54	0
56	MG	10	104	1/1	0.98	0.04	55,55,55,55	0
56	MG	2A	3672	1/1	0.98	0.25	41,41,41,41	0
56	MG	1a	1678	1/1	0.98	0.14	57,57,57,57	0
56	MG	1a	1780	1/1	0.98	0.07	47,47,47,47	0
56	MG	1A	3127	1/1	0.98	0.18	47,47,47,47	0
56	MG	1B	3023	1/1	0.98	0.19	51,51,51,51	0
56	MG	1A	3339	1/1	0.98	0.23	46,46,46,46	0
56	MG	2A	3383	1/1	0.98	0.11	46,46,46,46	0
56	MG	2A	3018	1/1	0.98	0.26	52,52,52,52	0
56	MG	1A	3138	1/1	0.98	0.26	32,32,32,32	0
56	MG	1A	3005	1/1	0.98	0.15	43,43,43,43	0
56	MG	1A	3567	1/1	0.98	0.13	15,15,15,15	0
56	MG	1a	1787	1/1	0.98	0.14	48,48,48,48	0
56	MG	1A	3617	1/1	0.98	0.17	26,26,26,26	0
56	MG	1A	3342	1/1	0.98	0.27	33,33,33,33	0
56	MG	2A	3258	1/1	0.98	0.06	35,35,35,35	0
56	MG	2B	3012	1/1	0.98	0.19	51,51,51,51	0
56	MG	1A	3911	1/1	0.98	0.20	53,53,53,53	0
56	MG	1A	3841	1/1	0.98	0.18	22,22,22,22	0
56	MG	1A	3487	1/1	0.98	0.18	24,24,24,24	0
56	MG	1A	3298	1/1	0.98	0.21	33,33,33,33	0
56	MG	1A	3916	1/1	0.98	0.31	34,34,34,34	0
56	MG	1A	3672	1/1	0.98	0.08	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3265	1/1	0.98	0.11	51,51,51,51	0
56	MG	2A	3541	1/1	0.98	0.11	51,51,51,51	0
56	MG	1A	3621	1/1	0.98	0.12	48,48,48,48	0
56	MG	2A	3543	1/1	0.98	0.11	28,28,28,28	0
56	MG	2A	3267	1/1	0.98	0.17	53,53,53,53	0
56	MG	2a	1732	1/1	0.98	0.10	45,45,45,45	0
56	MG	1a	1797	1/1	0.98	0.19	52,52,52,52	0
56	MG	2E	305	1/1	0.98	0.13	39,39,39,39	0
56	MG	1E	303	1/1	0.98	0.12	26,26,26,26	0
56	MG	2A	3146	1/1	0.98	0.16	33,33,33,33	0
56	MG	2A	3147	1/1	0.98	0.12	38,38,38,38	0
56	MG	1A	3033	1/1	0.98	0.16	22,22,22,22	0
56	MG	1A	3454	1/1	0.98	0.20	35,35,35,35	0
56	MG	1A	3921	1/1	0.98	0.26	40,40,40,40	0
56	MG	1A	3922	1/1	0.98	0.15	41,41,41,41	0
56	MG	1A	3849	1/1	0.98	0.20	29,29,29,29	0
56	MG	2A	3410	1/1	0.98	0.10	43,43,43,43	0
56	MG	2Q	202	1/1	0.98	0.14	46,46,46,46	0
56	MG	2A	3411	1/1	0.98	0.23	50,50,50,50	0
56	MG	2A	3277	1/1	0.98	0.17	35,35,35,35	0
56	MG	2A	3153	1/1	0.98	0.14	42,42,42,42	0
56	MG	2A	3154	1/1	0.98	0.21	41,41,41,41	0
56	MG	1A	3924	1/1	0.98	0.26	28,28,28,28	0
56	MG	2U	202	1/1	0.98	0.09	35,35,35,35	0
56	MG	2A	3560	1/1	0.98	0.11	51,51,51,51	0
56	MG	2A	3417	1/1	0.98	0.12	43,43,43,43	0
56	MG	2A	3562	1/1	0.98	0.14	42,42,42,42	0
56	MG	2a	1754	1/1	0.98	0.08	67,67,67,67	0
56	MG	2A	3156	1/1	0.98	0.24	31,31,31,31	0
56	MG	2A	3157	1/1	0.98	0.10	29,29,29,29	0
56	MG	1F	304	1/1	0.98	0.32	37,37,37,37	0
56	MG	2A	3042	1/1	0.98	0.15	37,37,37,37	0
56	MG	1A	3676	1/1	0.98	0.25	50,50,50,50	0
56	MG	1A	3786	1/1	0.98	0.16	36,36,36,36	0
56	MG	1A	3928	1/1	0.98	0.13	24,24,24,24	0
56	MG	1A	3929	1/1	0.98	0.43	45,45,45,45	0
56	MG	2a	1763	1/1	0.98	0.16	46,46,46,46	0
56	MG	1A	3573	1/1	0.98	0.14	34,34,34,34	0
56	MG	2a	1602	1/1	0.98	0.25	60,60,60,60	0
56	MG	2A	3572	1/1	0.98	0.09	43,43,43,43	0
56	MG	1A	3012	1/1	0.98	0.16	28,28,28,28	0
56	MG	1A	3394	1/1	0.98	0.18	12,12,12,12	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3855	1/1	0.98	0.17	23,23,23,23	0
56	MG	1A	3395	1/1	0.98	0.20	31,31,31,31	0
56	MG	2A	3431	1/1	0.98	0.16	52,52,52,52	0
56	MG	2A	3432	1/1	0.98	0.12	36,36,36,36	0
56	MG	1A	3792	1/1	0.98	0.11	17,17,17,17	0
56	MG	1A	3425	1/1	0.98	0.17	36,36,36,36	0
56	MG	1a	1713	1/1	0.98	0.25	53,53,53,53	0
56	MG	1a	1619	1/1	0.98	0.09	56,56,56,56	0
56	MG	2A	3437	1/1	0.98	0.13	34,34,34,34	0
56	MG	2a	1778	1/1	0.98	0.05	51,51,51,51	0
56	MG	1A	3533	1/1	0.98	0.08	28,28,28,28	0
56	MG	2A	3174	1/1	0.98	0.08	42,42,42,42	0
56	MG	2A	3586	1/1	0.98	0.11	44,44,44,44	0
56	MG	1A	3860	1/1	0.98	0.14	38,38,38,38	0
56	MG	2A	3059	1/1	0.98	0.10	46,46,46,46	0
56	MG	2a	1784	1/1	0.98	0.11	56,56,56,56	0
56	MG	1A	3795	1/1	0.98	0.13	20,20,20,20	0
56	MG	1A	3346	1/1	0.98	0.20	41,41,41,41	0
56	MG	1A	3156	1/1	0.98	0.24	34,34,34,34	0
56	MG	1a	1720	1/1	0.98	0.17	64,64,64,64	0
56	MG	1A	3942	1/1	0.98	0.19	32,32,32,32	0
56	MG	1A	3536	1/1	0.98	0.11	48,48,48,48	0
56	MG	2A	3595	1/1	0.98	0.08	57,57,57,57	0
56	MG	2A	3183	1/1	0.98	0.08	44,44,44,44	0
56	MG	1A	3944	1/1	0.98	0.30	33,33,33,33	0
56	MG	1A	3064	1/1	0.98	0.20	35,35,35,35	0
56	MG	2a	1630	1/1	0.98	0.21	55,55,55,55	0
56	MG	1A	3400	1/1	0.98	0.14	28,28,28,28	0
56	MG	1a	1830	1/1	0.98	0.15	44,44,44,44	0
56	MG	1A	3186	1/1	0.98	0.35	56,56,56,56	0
56	MG	1A	3585	1/1	0.98	0.13	49,49,49,49	0
56	MG	1a	1728	1/1	0.98	0.15	49,49,49,49	0
56	MG	1A	3500	1/1	0.98	0.13	26,26,26,26	0
56	MG	2A	3317	1/1	0.98	0.15	38,38,38,38	0
56	MG	1a	1633	1/1	0.98	0.24	52,52,52,52	0
56	MG	2A	3460	1/1	0.98	0.12	40,40,40,40	0
56	MG	1A	3804	1/1	0.98	0.16	26,26,26,26	0
56	MG	1a	1732	1/1	0.98	0.26	42,42,42,42	0
56	MG	1A	3249	1/1	0.98	0.40	29,29,29,29	0
56	MG	1A	3433	1/1	0.98	0.18	42,42,42,42	0
56	MG	1A	3467	1/1	0.98	0.17	43,43,43,43	0
56	MG	1A	3010	1/1	0.98	0.15	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3956	1/1	0.98	0.26	35,35,35,35	0
56	MG	2A	3326	1/1	0.98	0.06	42,42,42,42	0
56	MG	1A	3695	1/1	0.98	0.26	42,42,42,42	0
56	MG	1A	3545	1/1	0.98	0.08	57,57,57,57	0
56	MG	2A	3329	1/1	0.98	0.07	43,43,43,43	0
56	MG	1A	3404	1/1	0.98	0.14	44,44,44,44	0
56	MG	2A	3331	1/1	0.98	0.20	39,39,39,39	0
56	MG	1A	3547	1/1	0.98	0.08	36,36,36,36	0
56	MG	1A	3328	1/1	0.98	0.12	27,27,27,27	0
56	MG	1A	3202	1/1	0.98	0.33	31,31,31,31	0
59	ZN	1Y	501	1/1	0.98	0.18	67,67,67,67	0
56	MG	1A	3472	1/1	0.98	0.17	32,32,32,32	0
59	ZN	19	103	1/1	0.98	0.26	61,61,61,61	0
59	ZN	1n	501	1/1	0.98	0.16	58,58,58,58	0
56	MG	1A	3551	1/1	0.98	0.18	26,26,26,26	0
56	MG	2A	3479	1/1	0.98	0.11	39,39,39,39	0
56	MG	1A	3965	1/1	0.98	0.28	38,38,38,38	0
56	MG	1U	203	1/1	0.98	0.27	27,27,27,27	0
60	SF4	1d	501	8/8	0.98	0.16	55,66,73,80	0
60	SF4	2d	301	8/8	0.98	0.12	51,72,83,98	0
56	MG	1B	3001	1/1	0.98	0.25	39,39,39,39	0
56	MG	2A	3342	1/1	0.98	0.22	31,31,31,31	0
56	MG	1A	3141	1/1	0.99	0.25	27,27,27,27	0
56	MG	1A	3791	1/1	0.99	0.18	43,43,43,43	0
56	MG	2A	3045	1/1	0.99	0.17	36,36,36,36	0
56	MG	2A	3335	1/1	0.99	0.09	25,25,25,25	0
56	MG	2A	3336	1/1	0.99	0.08	47,47,47,47	0
56	MG	1A	3398	1/1	0.99	0.19	27,27,27,27	0
56	MG	1A	3862	1/1	0.99	0.11	19,19,19,19	0
56	MG	1A	3596	1/1	0.99	0.16	32,32,32,32	0
56	MG	2A	3189	1/1	0.99	0.20	31,31,31,31	0
56	MG	2A	3021	1/1	0.99	0.19	38,38,38,38	0
56	MG	1A	3845	1/1	0.99	0.25	47,47,47,47	0
56	MG	1A	3925	1/1	0.99	0.07	59,59,59,59	0
56	MG	1A	3172	1/1	0.99	0.12	32,32,32,32	0
56	MG	1A	3146	1/1	0.99	0.22	31,31,31,31	0
56	MG	2A	3254	1/1	0.99	0.16	38,38,38,38	0
56	MG	1A	3949	1/1	0.99	0.27	28,28,28,28	0
56	MG	1G	204	1/1	0.99	0.03	48,48,48,48	0
56	MG	1A	3318	1/1	0.99	0.18	53,53,53,53	0
56	MG	1a	1767	1/1	0.99	0.24	67,67,67,67	0
56	MG	2A	3415	1/1	0.99	0.16	30,30,30,30	0

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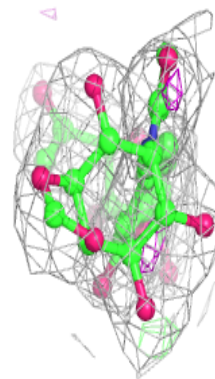
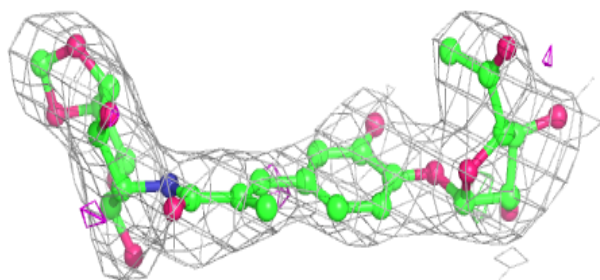
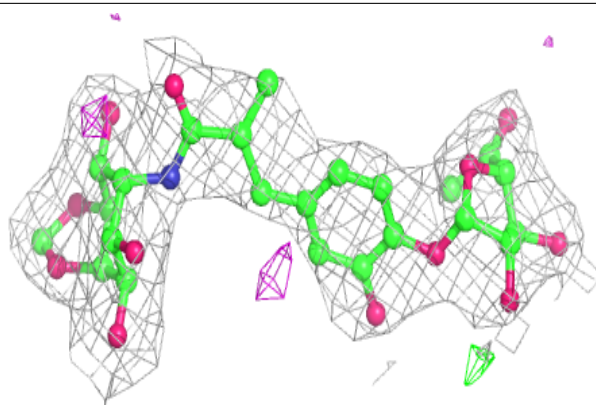
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3586	1/1	0.99	0.17	41,41,41,41	0
56	MG	1A	3781	1/1	0.99	0.13	23,23,23,23	0
56	MG	1a	1770	1/1	0.99	0.14	44,44,44,44	0
56	MG	1N	3003	1/1	0.99	0.17	36,36,36,36	0
56	MG	1A	3432	1/1	0.99	0.21	22,22,22,22	0
56	MG	2A	3454	1/1	0.99	0.09	36,36,36,36	0
56	MG	1A	3126	1/1	0.99	0.36	39,39,39,39	0
59	ZN	15	101	1/1	0.99	0.12	25,25,25,25	0
59	ZN	16	501	1/1	0.99	0.20	35,35,35,35	0
56	MG	2D	302	1/1	0.99	0.10	27,27,27,27	0
56	MG	1A	3032	1/1	0.99	0.21	41,41,41,41	0
56	MG	2D	304	1/1	0.99	0.23	42,42,42,42	0
56	MG	1A	3149	1/1	0.99	0.30	30,30,30,30	0
59	ZN	25	101	1/1	0.99	0.18	64,64,64,64	0
59	ZN	26	501	1/1	0.99	0.19	54,54,54,54	0
56	MG	1A	3162	1/1	0.99	0.64	33,33,33,33	0
56	MG	1A	3606	1/1	0.99	0.17	19,19,19,19	0
56	MG	1A	3459	1/1	0.99	0.15	40,40,40,40	0
56	MG	2a	1645	1/1	0.99	0.15	50,50,50,50	0
56	MG	1A	3896	1/1	0.99	0.20	13,13,13,13	0
56	MG	1A	3024	1/1	0.99	0.17	27,27,27,27	0

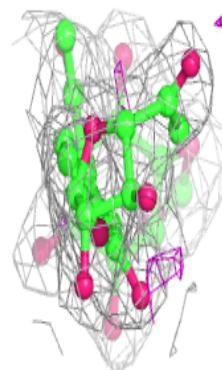
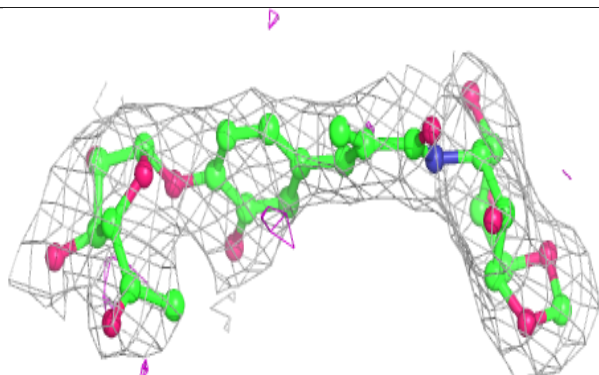
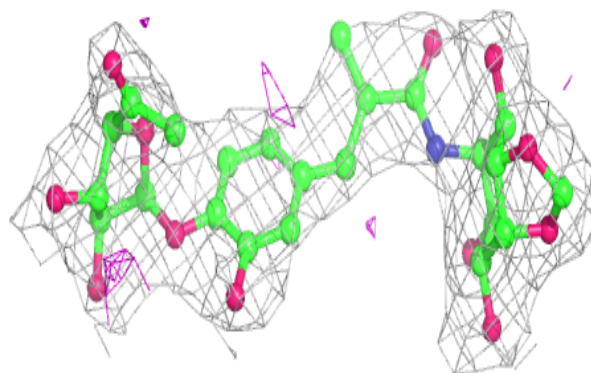
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HGR 2A 3652:

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

**Electron density around HGR 1A 3915:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.