Full wwPDB X-ray Structure Validation Report ⓘ

Nov 5, 2023 – 11:59 AM EST

PDB ID	:	8EV7
Title	:	Crystal structure of the Thermus thermophilus 70S ribosome in complex with kanamycin, mRNA, and A-, P-, and E-site tRNAs
Authors	:	Seely, S.M.; Gagnon, M.G.
Deposited on	:	2022-10-19
Resolution	:	2.89 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

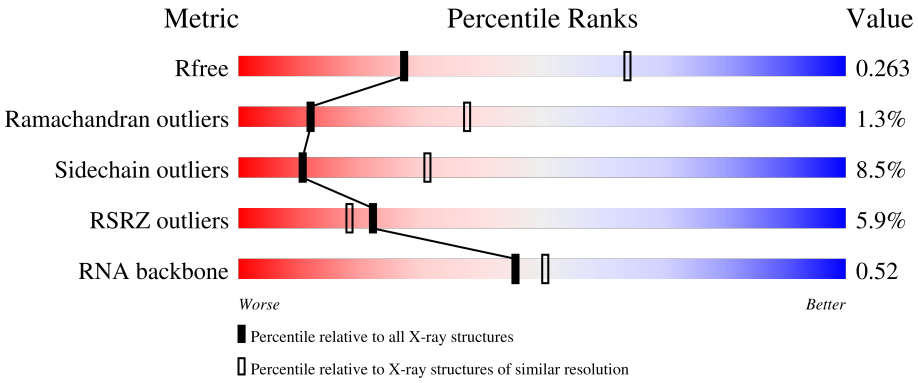
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 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	1957 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)
RNA backbone	3102	1007 (3.16-2.64)

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 <=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	82% 16%
1	2A	2915	78% 17%
2	1B	121	91% 7%
2	2B	121	70% 29%
3	1D	276	93% 7%

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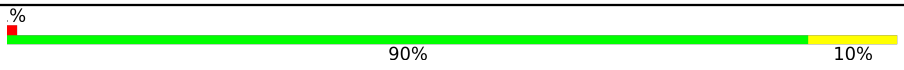
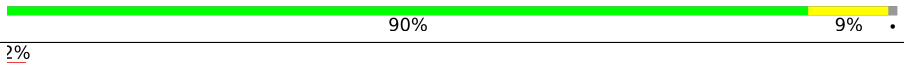
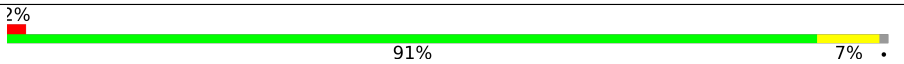
Mol	Chain	Length	Quality of chain
3	2D	276	
4	1E	206	
4	2E	206	
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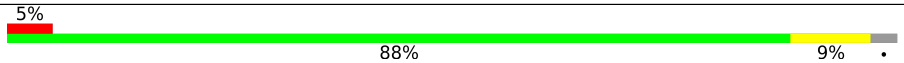
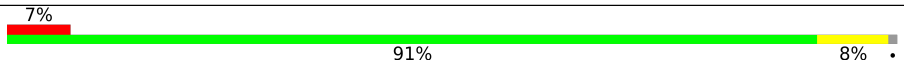
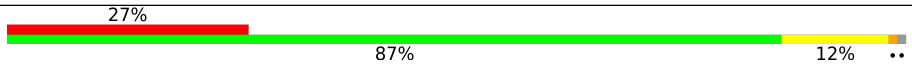
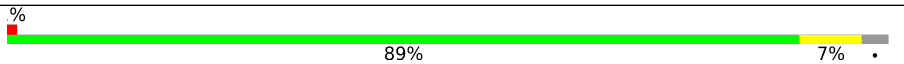
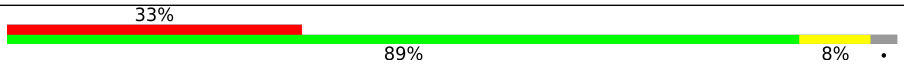
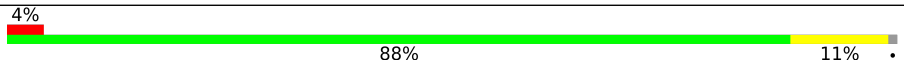
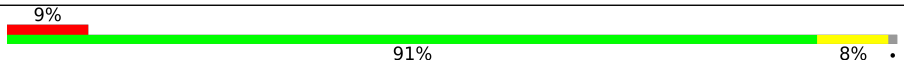
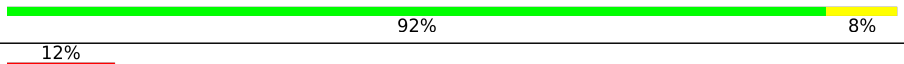
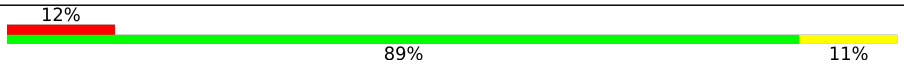
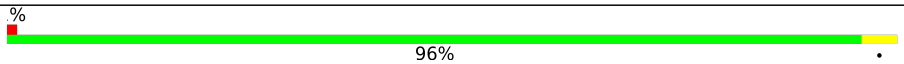
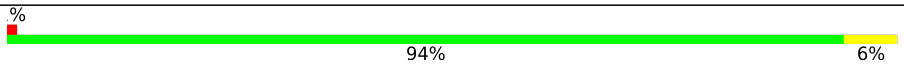
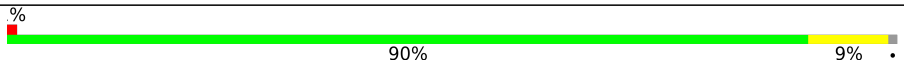
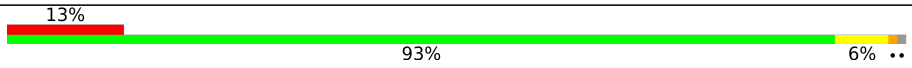
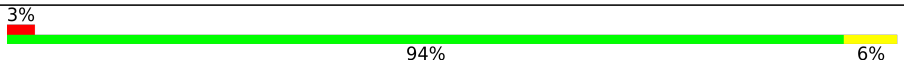
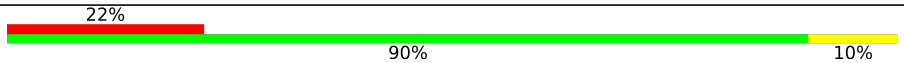
5	2F	210	
6	1G	182	
6	2G	182	
7	1H	180	
7	2H	180	
8	1I	148	
8	2I	148	
9	1N	140	
9	2N	140	
10	1O	122	
10	2O	122	
11	1P	150	
11	2P	150	
12	1Q	141	
12	2Q	141	
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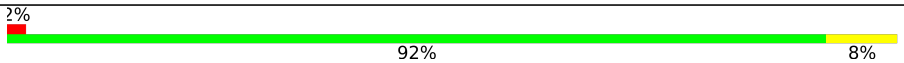
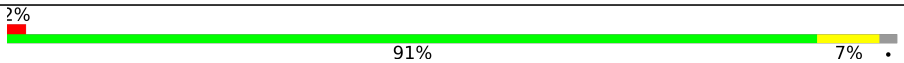
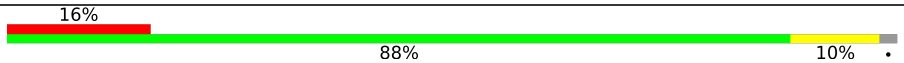
13	2R	118	
14	1S	112	
14	2S	112	
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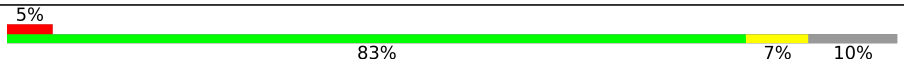
15	2T	146	

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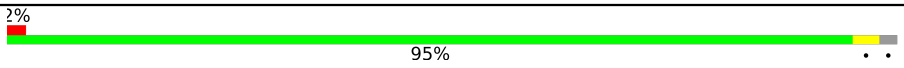
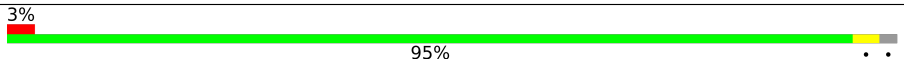
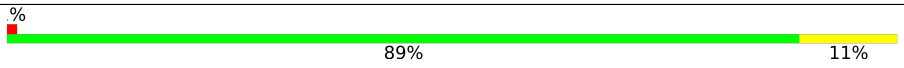
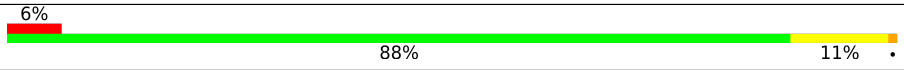
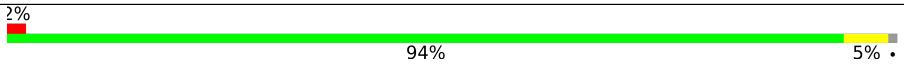
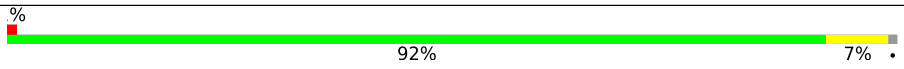
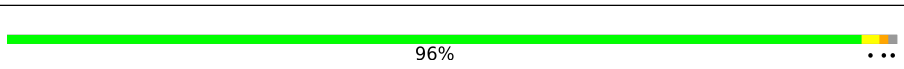
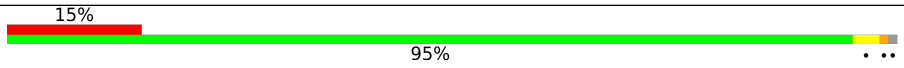
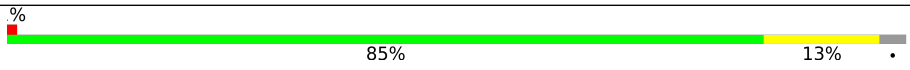
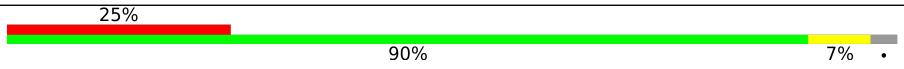
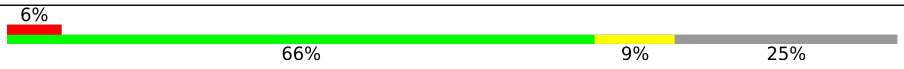
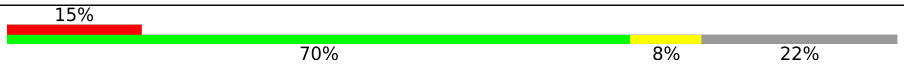
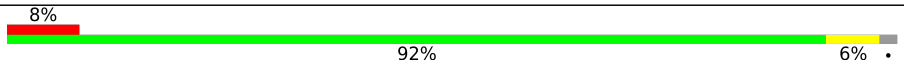
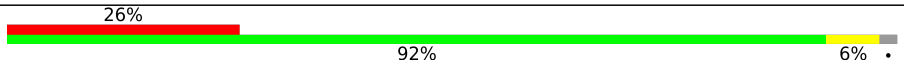
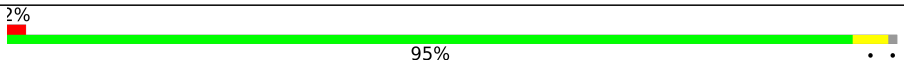
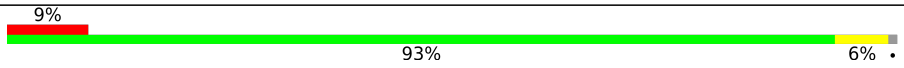
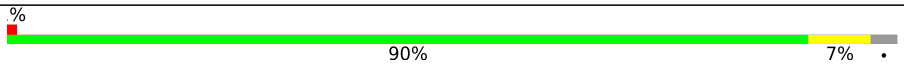
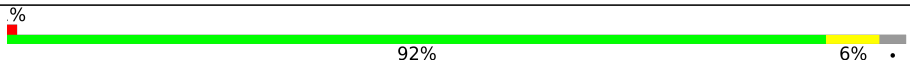
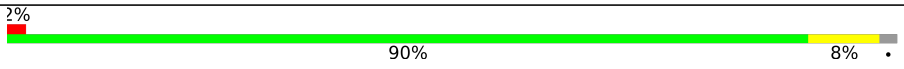
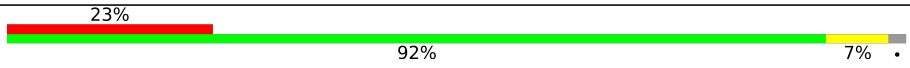
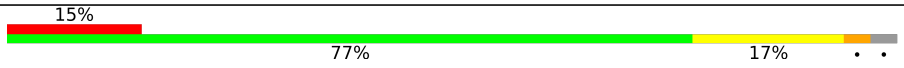
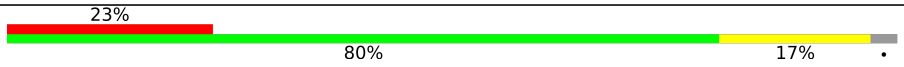
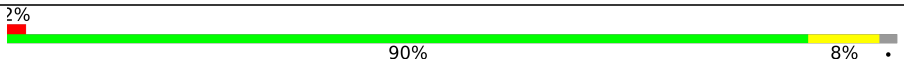
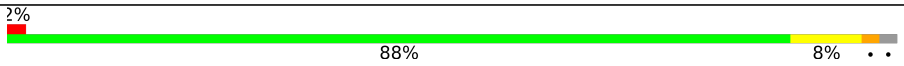
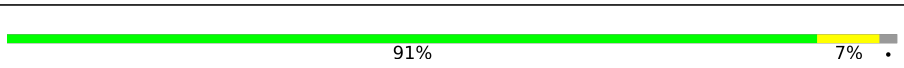
Mol	Chain	Length	Quality of chain
16	1U	118	
16	2U	118	
17	1V	101	
17	2V	101	
18	1W	113	
18	2W	113	
19	1X	96	
19	2X	96	
20	1Y	110	
20	2Y	110	
21	1Z	206	
21	2Z	206	
22	10	85	
22	20	85	
23	11	98	
23	21	98	
24	12	72	
24	22	72	
25	13	60	
25	23	60	
26	14	71	
26	24	71	
27	15	60	
27	25	60	
28	16	54	

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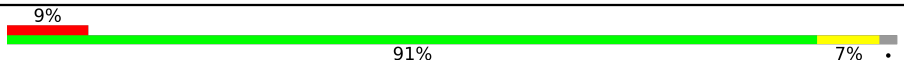
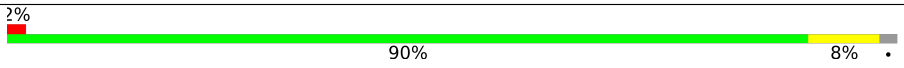
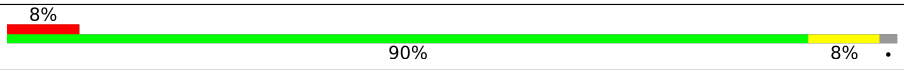
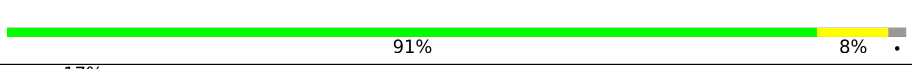
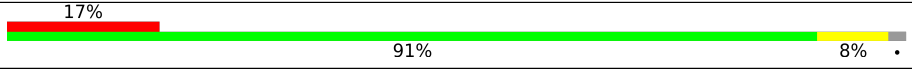
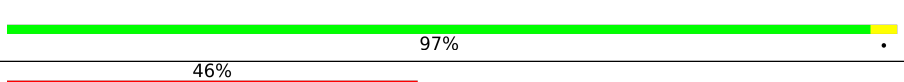
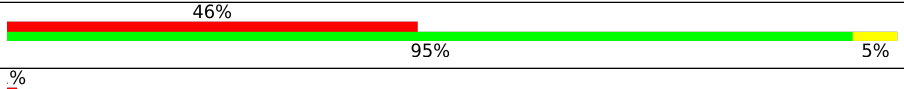
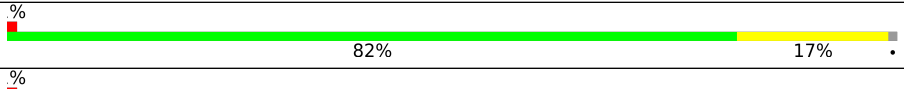
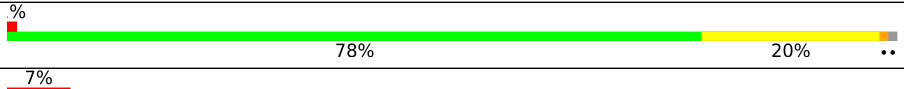
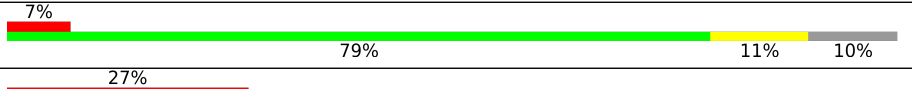
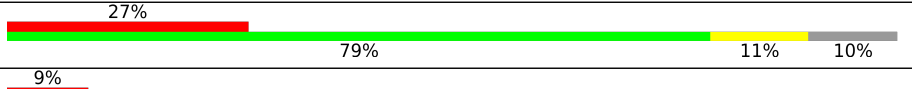
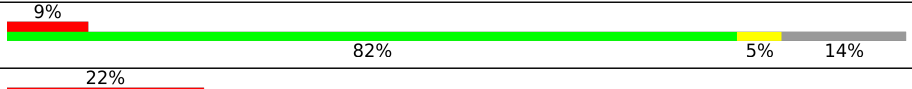
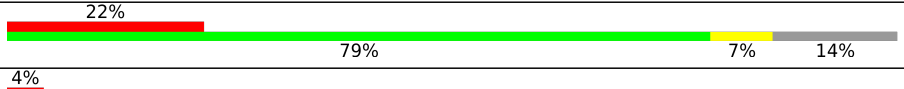
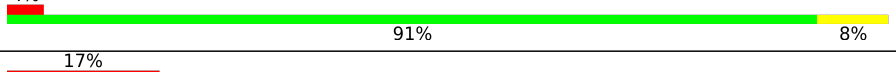
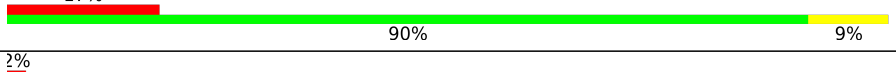
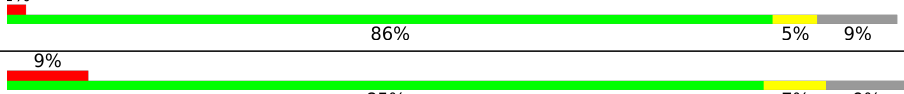
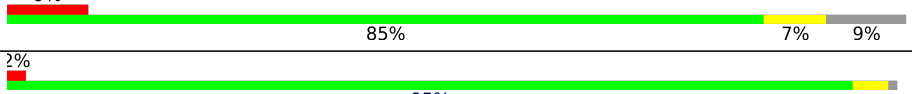
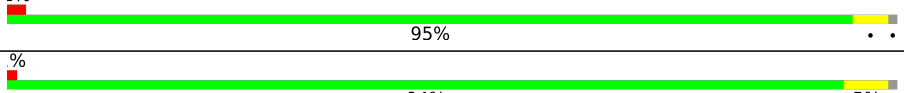
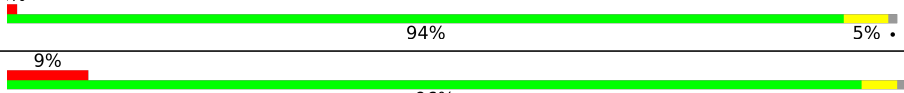
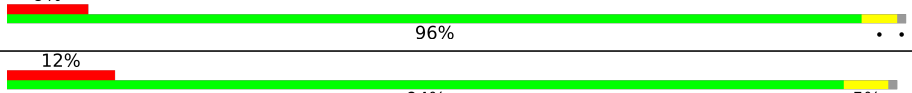
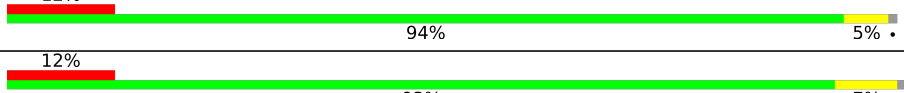
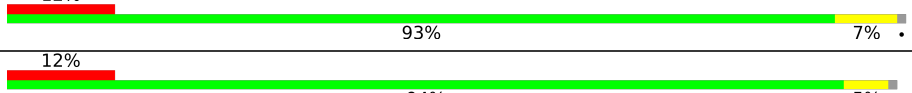
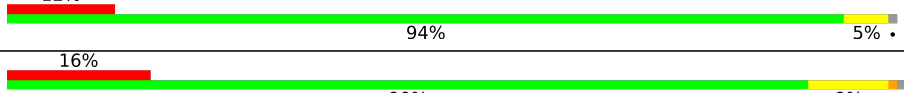
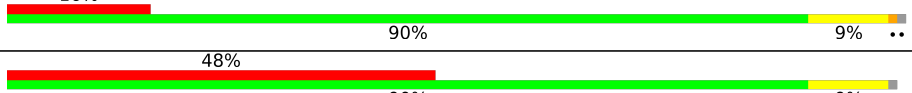
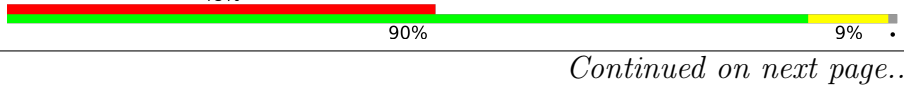
Mol	Chain	Length	Quality of chain
28	26	54	
29	17	49	
29	27	49	
30	18	65	
30	28	65	
31	19	37	
31	29	37	
32	1a	1521	
32	2a	1521	
33	1b	256	
33	2b	256	
34	1c	239	
34	2c	239	
35	1d	209	
35	2d	209	
36	1e	162	
36	2e	162	
37	1f	101	
37	2f	101	
38	1g	156	
38	2g	156	
39	1h	138	
39	2h	138	
40	1i	128	
40	2i	128	

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Mol	Chain	Length	Quality of chain
41	1j	105	11% 86% 7% 8%
41	2j	105	25% 84% 8% 9%
42	1k	129	3% 80% 9% 12%
42	2k	129	14% 84% 5% 12%
43	1l	132	% 86% 7% 8%
43	2l	132	8% 86% 7% 8%
44	1m	126	6% 90% 8%
44	2m	126	23% 90% 7%
45	1n	61	10% 89% 10%
45	2n	61	49% 87% 11%
46	1o	89	% 90% 9%
46	2o	89	4% 93% 6%
47	1p	88	11% 88% 6% 7%
47	2p	88	19% 82% 10% 7%
48	1q	105	2% 89% 6% 6%
48	2q	105	14% 90% 5% 6%
49	1r	88	2% 69% 8% 23%
49	2r	88	8% 72% 6% 23%
50	1s	93	3% 82% 8% 11%
50	2s	93	9% 76% 13% 11%
51	1t	106	10% 83% 7% 9%
51	2t	106	13% 84% 7% 9%
52	1u	27	19% 85% 15%
52	2u	27	48% 81% 15%
53	1v	24	4% 50% 46%

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Mol	Chain	Length	Quality of chain
53	2v	24	17% 38% 17% 46%
54	1w	76	9% 59% 32% 7%
54	1y	76	5% 57% 36% 5%
54	2w	76	16% 55% 37% 5%
54	2y	76	8% 54% 39%
55	1x	77	78% 19%
55	2x	77	71% 27%

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	10	101	-	-	-	X
56	MG	1A	3011	-	-	-	X
56	MG	1A	3029	-	-	-	X
56	MG	1A	3121	-	-	-	X
56	MG	1A	3138	-	-	-	X
56	MG	1A	3154	-	-	-	X
56	MG	1A	3165	-	-	-	X
56	MG	1A	3166	-	-	-	X
56	MG	1A	3167	-	-	-	X
56	MG	1A	3168	-	-	-	X
56	MG	1A	3187	-	-	-	X
56	MG	1A	3196	-	-	-	X
56	MG	1A	3202	-	-	-	X
56	MG	1A	3218	-	-	-	X
56	MG	1A	3227	-	-	-	X
56	MG	1A	3229	-	-	-	X
56	MG	1A	3252	-	-	-	X
56	MG	1A	3299	-	-	-	X
56	MG	1A	3358	-	-	-	X
56	MG	1A	3402	-	-	-	X
56	MG	1A	3403	-	-	-	X
56	MG	1A	3422	-	-	-	X
56	MG	1A	3558	-	-	-	X
56	MG	1A	3615	-	-	-	X
56	MG	1A	3658	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1A	3761	-	-	-	X
56	MG	1A	3770	-	-	-	X
56	MG	1A	3784	-	-	-	X
56	MG	1A	3792	-	-	-	X
56	MG	1A	3837	-	-	-	X
56	MG	1A	3845	-	-	-	X
56	MG	1A	3850	-	-	-	X
56	MG	1A	3856	-	-	-	X
56	MG	1A	3929	-	-	-	X
56	MG	1B	220	-	-	-	X
56	MG	1D	302	-	-	-	X
56	MG	1a	1609	-	-	-	X
56	MG	1a	1615	-	-	-	X
56	MG	1a	1618	-	-	-	X
56	MG	1a	1713	-	-	-	X
56	MG	1a	1745	-	-	-	X
56	MG	1a	1749	-	-	-	X
56	MG	1a	1769	-	-	-	X
56	MG	1a	1792	-	-	-	X
56	MG	1a	1881	-	-	-	X
56	MG	1a	1883	-	-	-	X
56	MG	1a	1912	-	-	-	X
56	MG	1a	1924	-	-	-	X
56	MG	1e	201	-	-	-	X
56	MG	1w	104	-	-	-	X
56	MG	20	102	-	-	-	X
56	MG	23	101	-	-	-	X
56	MG	2A	3038	-	-	-	X
56	MG	2A	3061	-	-	-	X
56	MG	2A	3159	-	-	-	X
56	MG	2A	3332	-	-	-	X
56	MG	2A	3333	-	-	-	X
56	MG	2A	3360	-	-	-	X
56	MG	2A	3378	-	-	-	X
56	MG	2A	3433	-	-	-	X
56	MG	2A	3447	-	-	-	X
56	MG	2A	3451	-	-	-	X
56	MG	2A	3456	-	-	-	X
56	MG	2A	3496	-	-	-	X
56	MG	2A	3513	-	-	-	X
56	MG	2A	3524	-	-	-	X
56	MG	2A	3532	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	2T	202	-	-	-	X
56	MG	2a	1605	-	-	-	X
56	MG	2a	1678	-	-	-	X
56	MG	2a	1679	-	-	-	X
56	MG	2a	1705	-	-	-	X
56	MG	2a	1725	-	-	-	X
56	MG	2a	1730	-	-	-	X
56	MG	2a	1773	-	-	-	X
56	MG	2a	1782	-	-	-	X

2 Entry composition (i)

There are 60 unique types of molecules in this entry. The entry contains 297628 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	1F	203	Total	C	N	O	S	0	0	1
			1584	1009	298	275	2			
5	2F	203	Total	C	N	O	S	0	0	1
			1580	1007	297	274	2			

- Molecule 6 is a protein called 50S ribosomal protein L5.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 53 is a RNA chain called mRNA.

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
54	1w	74	Total	C	N	O	P	S	0	0	0
			1592	713	285	518	74	2			
54	1y	74	Total	C	N	O	P	S	0	0	0
			1585	707	285	518	74	1			
54	2w	72	Total	C	N	O	P	S	0	0	0
			1544	690	278	502	72	2			
54	2y	73	Total	C	N	O	P	S	0	0	0
			1565	698	283	510	73	1			

- 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	932	Total	Mg	0	0
			932	932		
56	1B	29	Total	Mg	0	0
			29	29		
56	1D	4	Total	Mg	0	0
			4	4		
56	1E	4	Total	Mg	0	0
			4	4		
56	1F	3	Total	Mg	0	0
			3	3		
56	1G	2	Total	Mg	0	0
			2	2		
56	1N	2	Total	Mg	0	0
			2	2		
56	1O	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	1P	2	Total Mg 2 2	0	0
56	1Q	3	Total Mg 3 3	0	0
56	1R	1	Total Mg 1 1	0	0
56	1T	1	Total Mg 1 1	0	0
56	1U	2	Total Mg 2 2	0	0
56	1V	2	Total Mg 2 2	0	0
56	1W	2	Total Mg 2 2	0	0
56	1X	1	Total Mg 1 1	0	0
56	1Y	1	Total Mg 1 1	0	0
56	10	1	Total Mg 1 1	0	0
56	11	1	Total Mg 1 1	0	0
56	12	1	Total Mg 1 1	0	0
56	13	4	Total Mg 4 4	0	0
56	14	1	Total Mg 1 1	0	0
56	15	3	Total Mg 3 3	0	0
56	16	1	Total Mg 1 1	0	0
56	17	1	Total Mg 1 1	0	0
56	18	4	Total Mg 4 4	0	0
56	19	3	Total Mg 3 3	0	0
56	1a	354	Total Mg 354 354	0	0
56	1d	2	Total Mg 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	1e	1	Total Mg 1 1	0	0
56	1i	1	Total Mg 1 1	0	0
56	1k	1	Total Mg 1 1	0	0
56	1l	3	Total Mg 3 3	0	0
56	1m	2	Total Mg 2 2	0	0
56	1o	3	Total Mg 3 3	0	0
56	1q	2	Total Mg 2 2	0	0
56	1r	1	Total Mg 1 1	0	0
56	1v	3	Total Mg 3 3	0	0
56	1w	5	Total Mg 5 5	0	0
56	1x	24	Total Mg 24 24	0	0
56	1y	1	Total Mg 1 1	0	0
56	2A	567	Total Mg 567 567	0	0
56	2B	13	Total Mg 13 13	0	0
56	2D	3	Total Mg 3 3	0	0
56	2E	2	Total Mg 2 2	0	0
56	2F	4	Total Mg 4 4	0	0
56	2G	1	Total Mg 1 1	0	0
56	2Q	2	Total Mg 2 2	0	0
56	2T	2	Total Mg 2 2	0	0
56	2W	1	Total Mg 1 1	0	0

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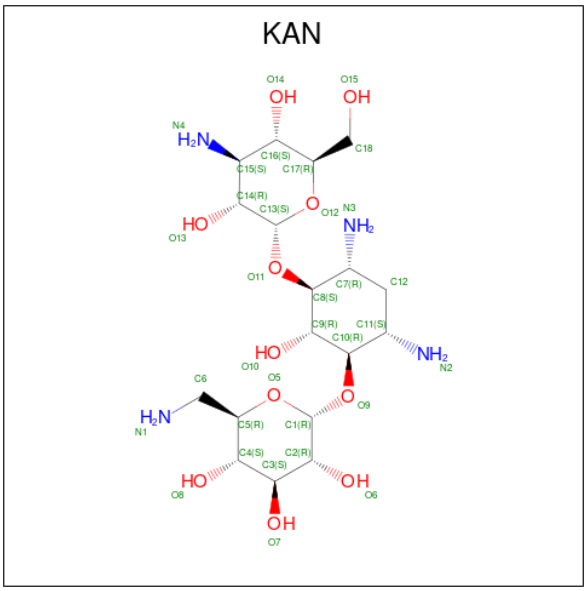
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	20	2	Total Mg 2 2	0	0
56	21	1	Total Mg 1 1	0	0
56	23	1	Total Mg 1 1	0	0
56	26	1	Total Mg 1 1	0	0
56	28	2	Total Mg 2 2	0	0
56	2a	227	Total Mg 227 227	0	0
56	2e	1	Total Mg 1 1	0	0
56	2g	1	Total Mg 1 1	0	0
56	2q	1	Total Mg 1 1	0	0
56	2t	1	Total Mg 1 1	0	0
56	2v	2	Total Mg 2 2	0	0
56	2w	1	Total Mg 1 1	0	0
56	2x	7	Total Mg 7 7	0	0

- Molecule 57 is KANAMYCIN A (three-letter code: KAN) (formula: $C_{18}H_{36}N_4O_{11}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	1A	1	Total C N O 33 18 4 11	0	0
57	1A	1	Total C N O 33 18 4 11	0	0
57	1A	1	Total C N O 33 18 4 11	0	0
57	1a	1	Total C N O 33 18 4 11	0	0
57	2A	1	Total C N O 33 18 4 11	0	0
57	2A	1	Total C N O 33 18 4 11	0	0
57	2a	1	Total C N O 33 18 4 11	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	1Y	1	Total Zn 1 1	0	0
58	14	1	Total Zn 1 1	0	0
58	15	1	Total Zn 1 1	0	0
58	16	1	Total Zn 1 1	0	0
58	19	1	Total Zn 1 1	0	0

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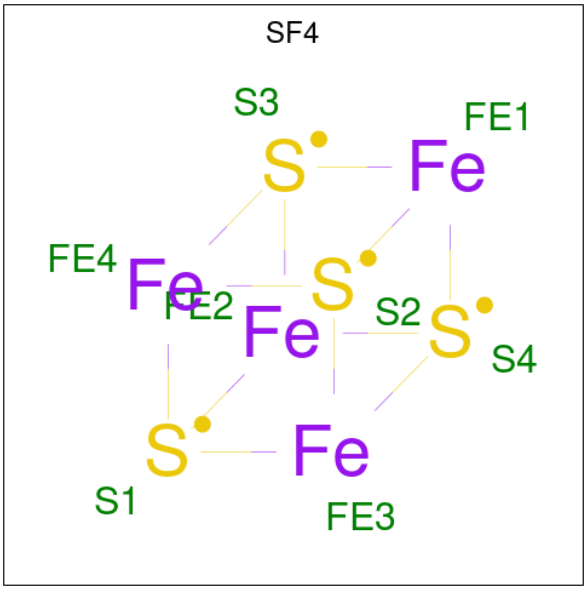
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	1n	1	Total Zn 1 1	0	0
58	2Y	1	Total Zn 1 1	0	0
58	24	1	Total Zn 1 1	0	0
58	25	1	Total Zn 1 1	0	0
58	26	1	Total Zn 1 1	0	0
58	29	1	Total Zn 1 1	0	0
58	2n	1	Total Zn 1 1	0	0

- Molecule 59 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

- Molecule 60 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	1A	938	Total O 938 938	0	0
60	1B	25	Total O 25 25	0	0
60	1D	9	Total O 9 9	0	0
60	1E	7	Total O 7 7	0	0
60	1F	9	Total O 9 9	0	0
60	1G	1	Total O 1 1	0	0
60	1H	1	Total O 1 1	0	0
60	1N	2	Total O 2 2	0	0
60	1O	4	Total O 4 4	0	0
60	1P	12	Total O 12 12	0	0
60	1Q	4	Total O 4 4	0	0
60	1R	5	Total O 5 5	0	0
60	1S	2	Total O 2 2	0	0
60	1T	8	Total O 8 8	0	0
60	1U	5	Total O 5 5	0	0
60	1V	4	Total O 4 4	0	0
60	1W	5	Total O 5 5	0	0
60	1X	4	Total O 4 4	0	0
60	1Y	5	Total O 5 5	0	0
60	1Z	1	Total O 1 1	0	0
60	10	4	Total O 4 4	0	0
60	11	4	Total O 4 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	12	2	Total O 2 2	0	0
60	13	1	Total O 1 1	0	0
60	14	1	Total O 1 1	0	0
60	15	1	Total O 1 1	0	0
60	16	3	Total O 3 3	0	0
60	17	3	Total O 3 3	0	0
60	18	2	Total O 2 2	0	0
60	19	1	Total O 1 1	0	0
60	1a	371	Total O 371 371	0	0
60	1d	4	Total O 4 4	0	0
60	1e	4	Total O 4 4	0	0
60	1f	2	Total O 2 2	0	0
60	1h	1	Total O 1 1	0	0
60	1i	2	Total O 2 2	0	0
60	1j	1	Total O 1 1	0	0
60	1k	1	Total O 1 1	0	0
60	1l	3	Total O 3 3	0	0
60	1m	2	Total O 2 2	0	0
60	1n	1	Total O 1 1	0	0
60	1o	3	Total O 3 3	0	0
60	1p	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	1s	1	Total O 1 1	0	0
60	1t	1	Total O 1 1	0	0
60	1v	3	Total O 3 3	0	0
60	1w	2	Total O 2 2	0	0
60	1x	16	Total O 16 16	0	0
60	2A	401	Total O 401 401	0	0
60	2B	18	Total O 18 18	0	0
60	2D	6	Total O 6 6	0	0
60	2E	3	Total O 3 3	0	0
60	2F	3	Total O 3 3	0	0
60	2O	1	Total O 1 1	0	0
60	2P	5	Total O 5 5	0	0
60	2R	2	Total O 2 2	0	0
60	2U	2	Total O 2 2	0	0
60	2W	1	Total O 1 1	0	0
60	2X	2	Total O 2 2	0	0
60	2Y	1	Total O 1 1	0	0
60	20	3	Total O 3 3	0	0
60	21	4	Total O 4 4	0	0
60	25	1	Total O 1 1	0	0
60	26	1	Total O 1 1	0	0

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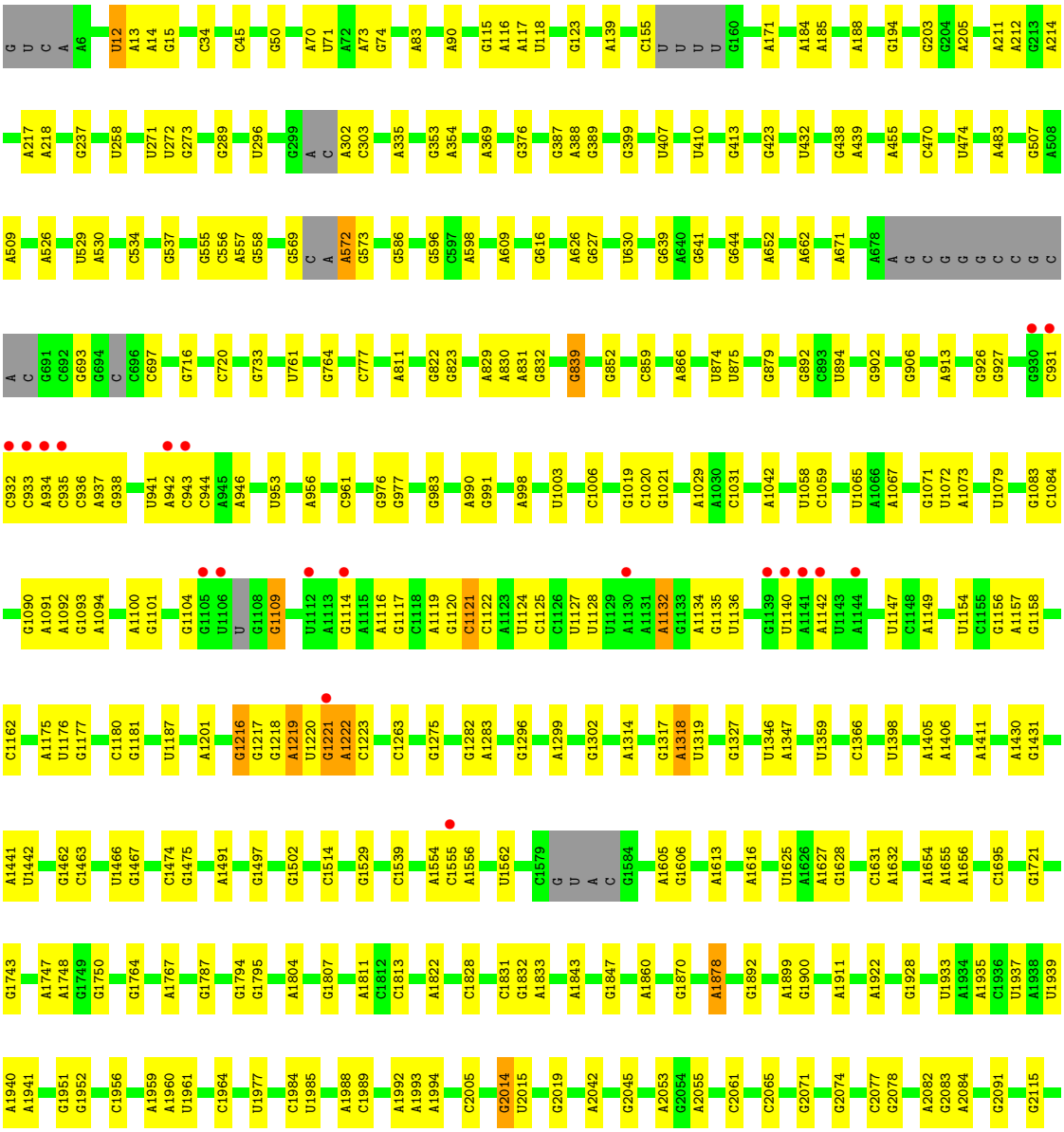
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	27	1	Total O 1 1	0	0
60	28	3	Total O 3 3	0	0
60	29	1	Total O 1 1	0	0
60	2a	160	Total O 160 160	0	0
60	2e	2	Total O 2 2	0	0
60	2i	1	Total O 1 1	0	0
60	2l	2	Total O 2 2	0	0
60	2m	2	Total O 2 2	0	0
60	2o	1	Total O 1 1	0	0
60	2t	3	Total O 3 3	0	0
60	2w	1	Total O 1 1	0	0
60	2x	2	Total O 2 2	0	0

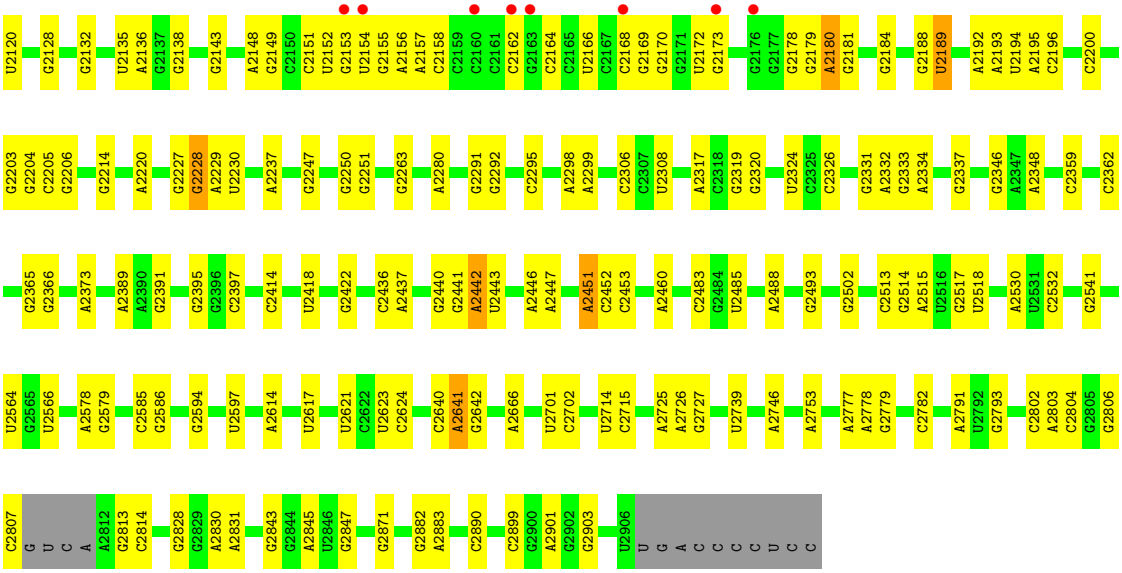
3 Residue-property plots (i)

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

- Molecule 1: 23S Ribosomal RNA

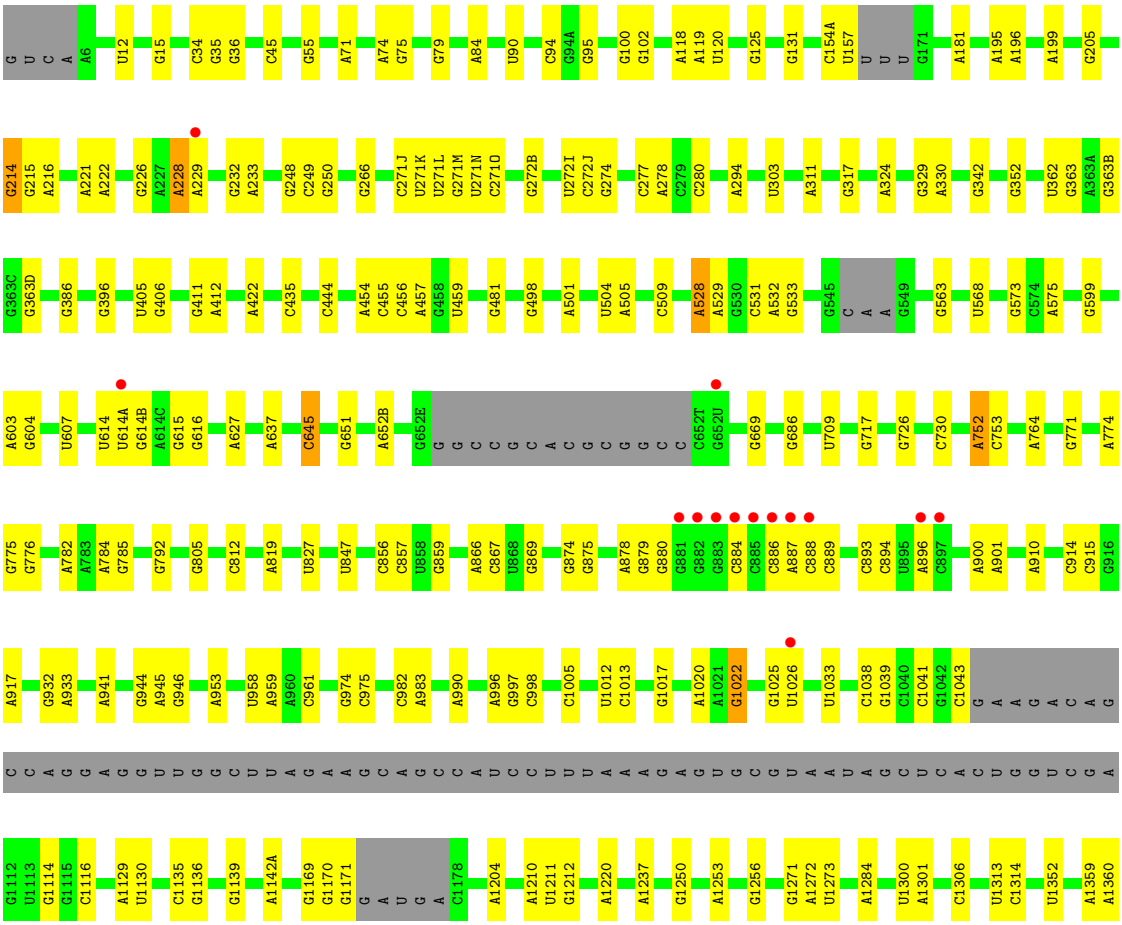
Chain 1A:

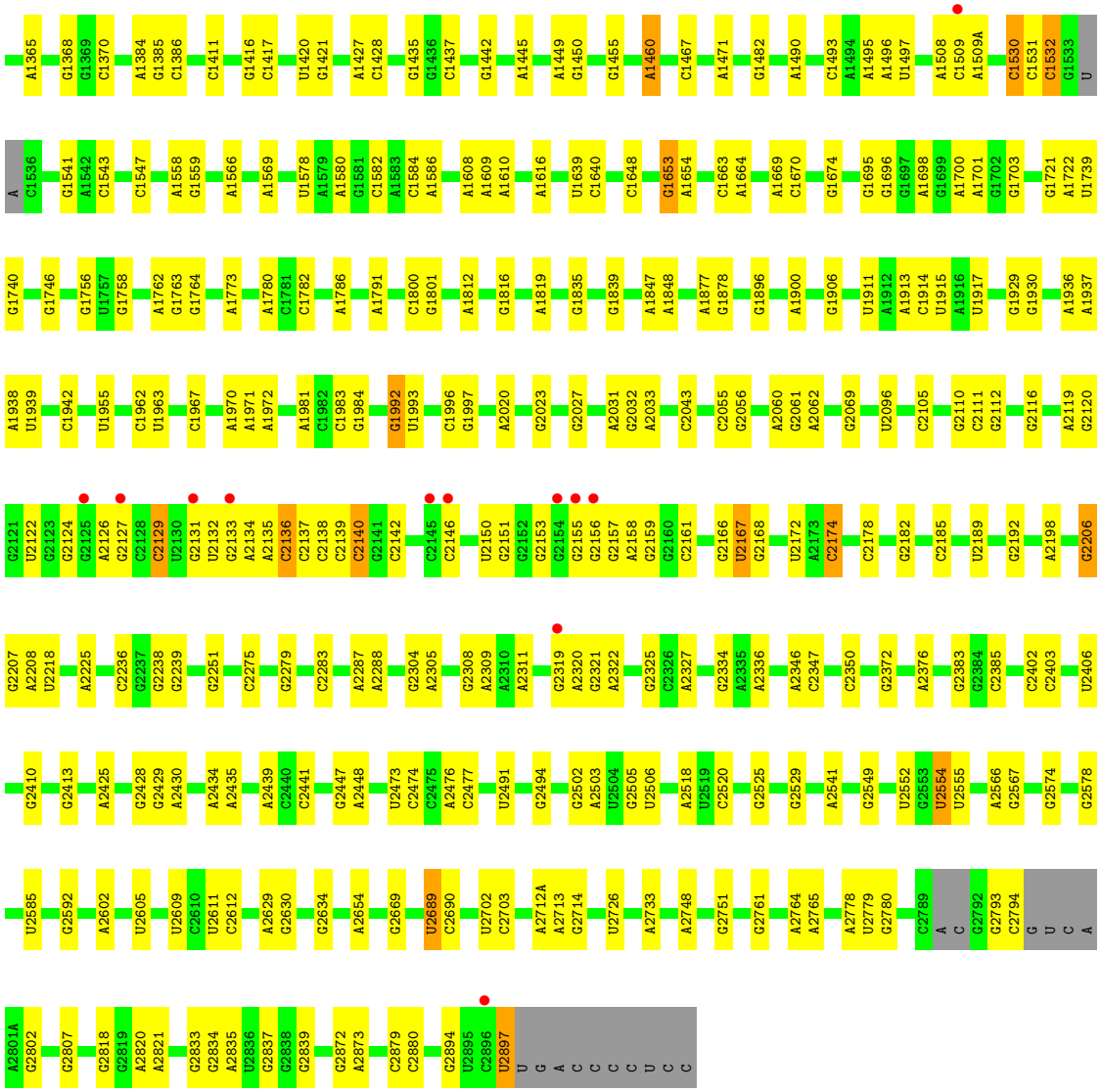




• Molecule 1: 23S Ribosomal RNA

Chain 2A:



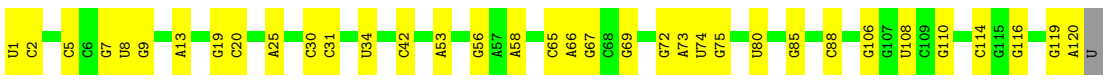


• Molecule 2: 5S Ribosomal RNA

Chain 1B:

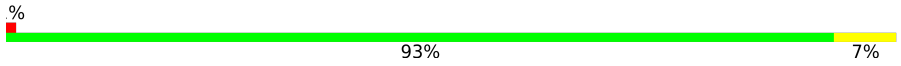
• Molecule 2: 5S Ribosomal RNA

Chain 2B:

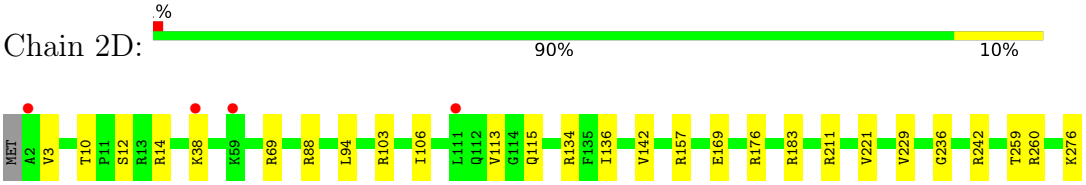


• Molecule 3: 50S ribosomal protein L2

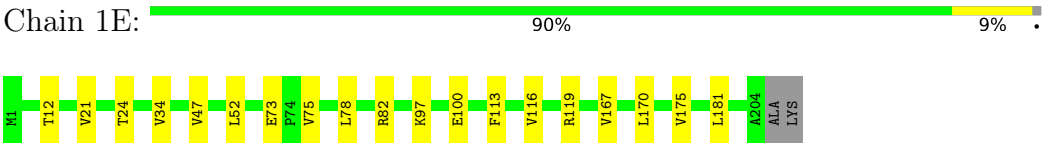
Chain 1D:



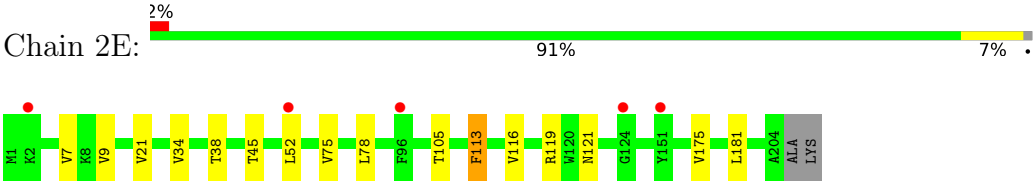
• Molecule 3: 50S ribosomal protein L2



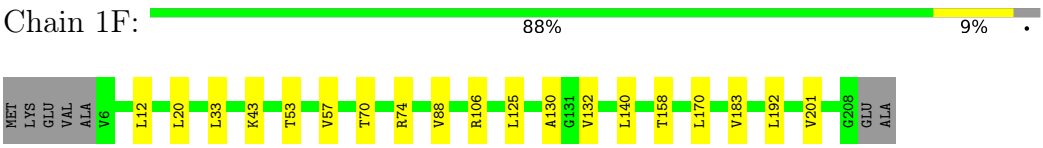
• Molecule 4: 50S ribosomal protein L3



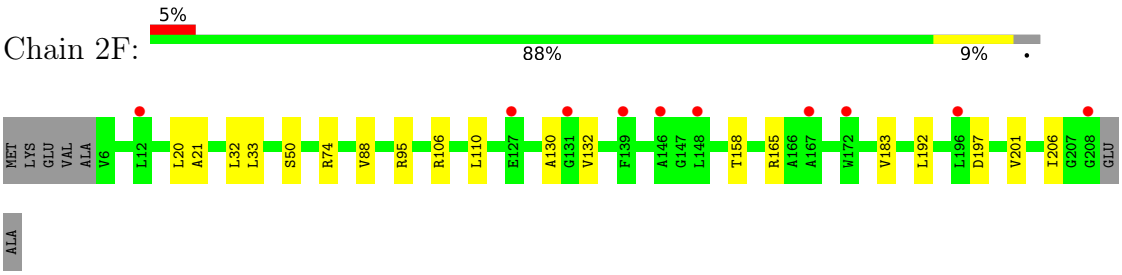
• Molecule 4: 50S ribosomal protein L3



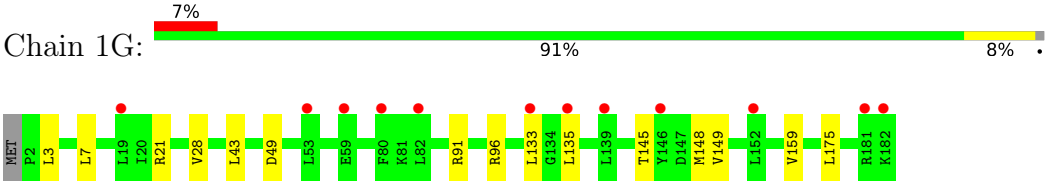
• Molecule 5: 50S ribosomal protein L4



• Molecule 5: 50S ribosomal protein L4

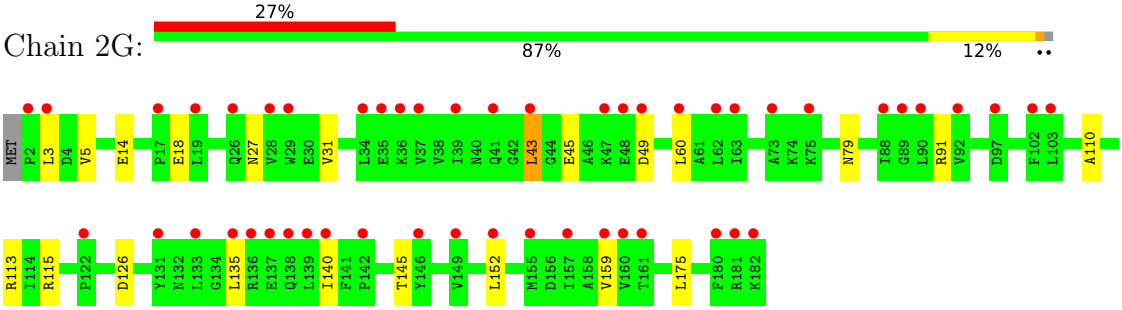


• Molecule 6: 50S ribosomal protein L5



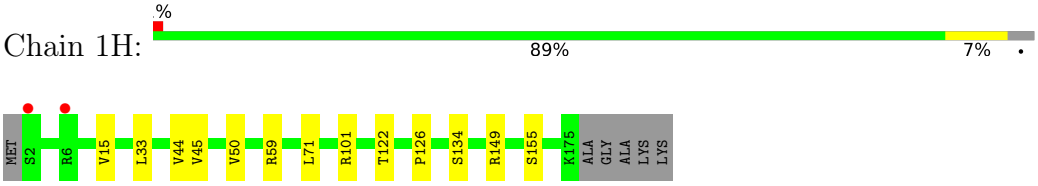
• Molecule 6: 50S ribosomal protein L5

Chain 2G:



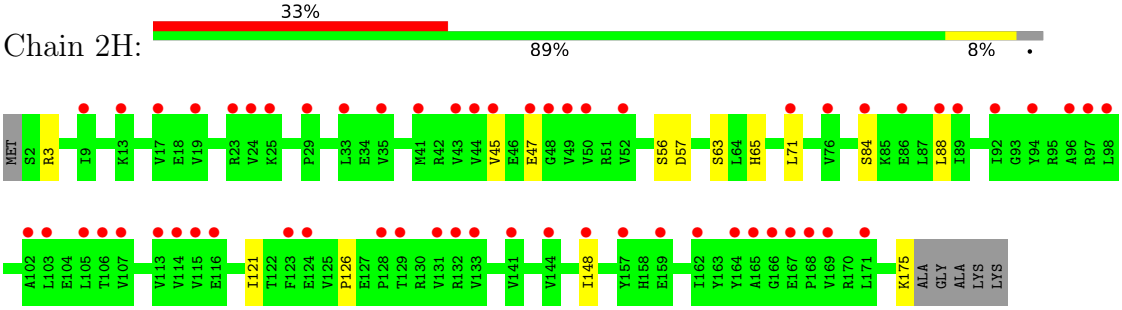
• Molecule 7: 50S ribosomal protein L6

Chain 1H:



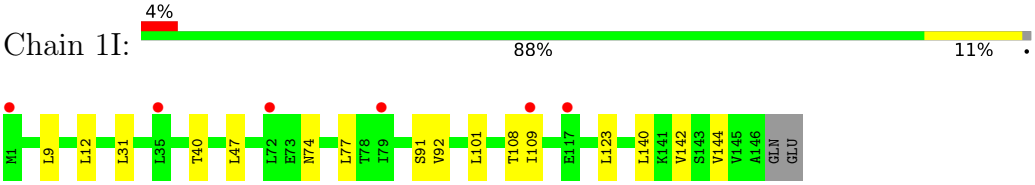
• Molecule 7: 50S ribosomal protein L6

Chain 2H:



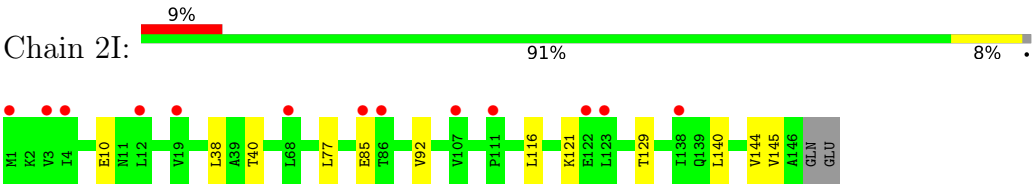
• Molecule 8: 50S ribosomal protein L9

Chain 1I:



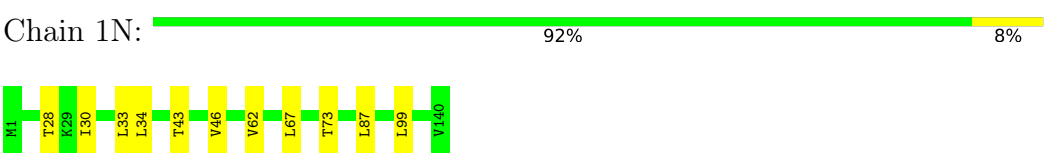
• Molecule 8: 50S ribosomal protein L9

Chain 2I:



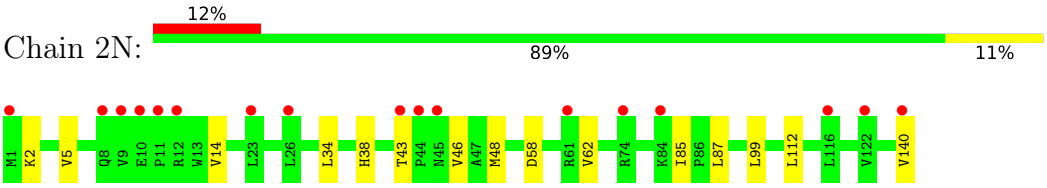
• Molecule 9: 50S ribosomal protein L13

Chain 1N:



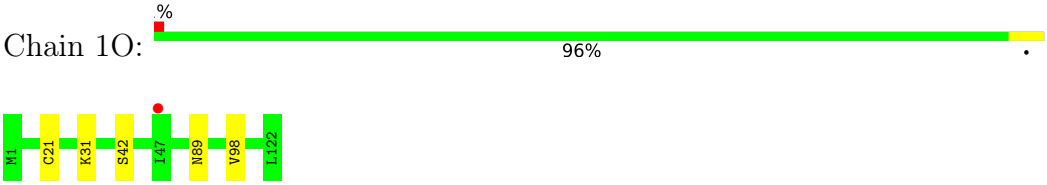
• Molecule 9: 50S ribosomal protein L13

Chain 2N:



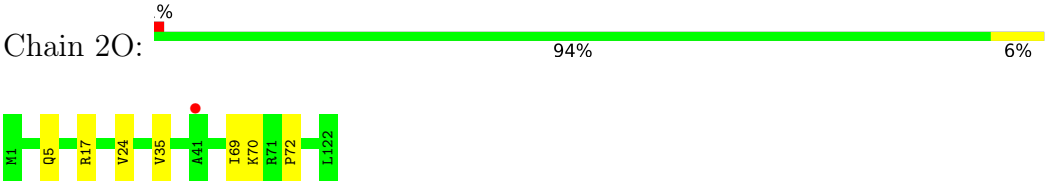
• Molecule 10: 50S ribosomal protein L14

Chain 1O:



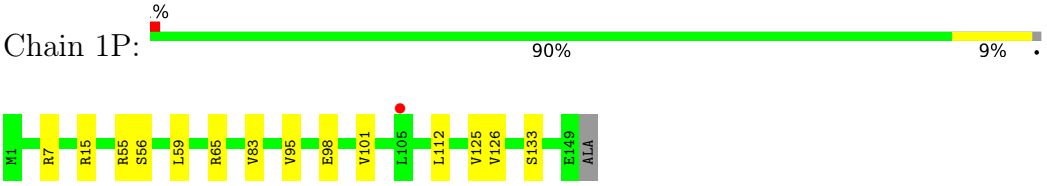
• Molecule 10: 50S ribosomal protein L14

Chain 2O:



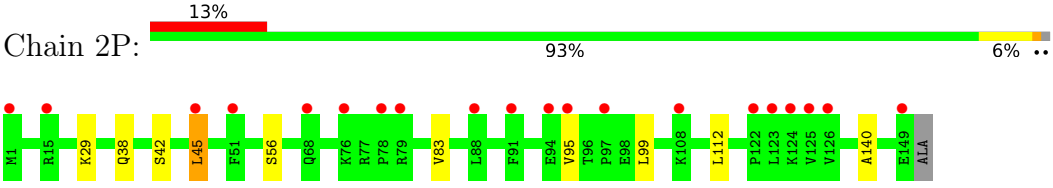
• Molecule 11: 50S ribosomal protein L15

Chain 1P:



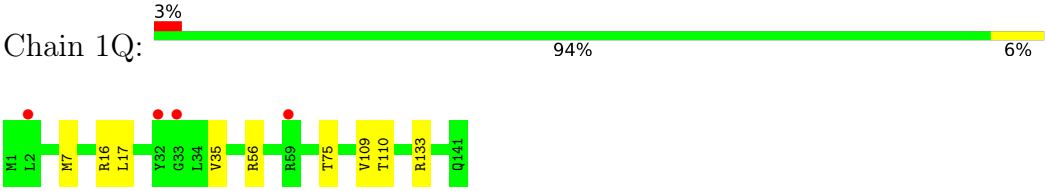
• Molecule 11: 50S ribosomal protein L15

Chain 2P:



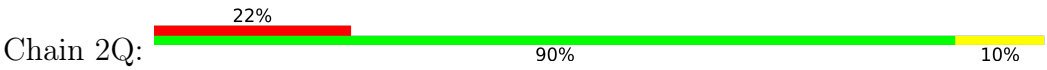
• Molecule 12: 50S ribosomal protein L16

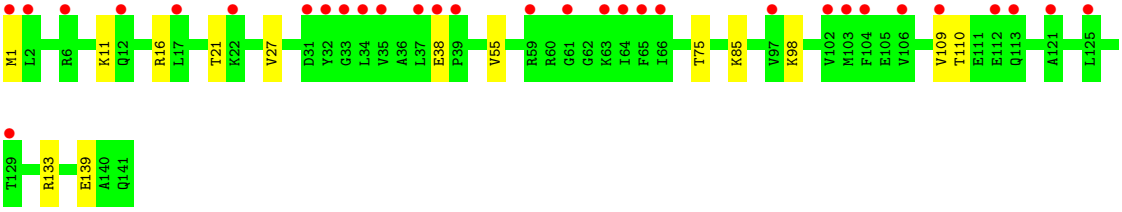
Chain 1Q:



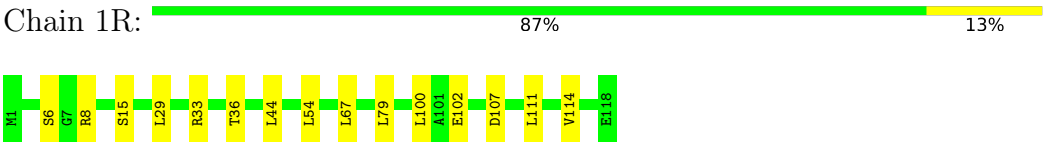
• Molecule 12: 50S ribosomal protein L16

Chain 2Q:

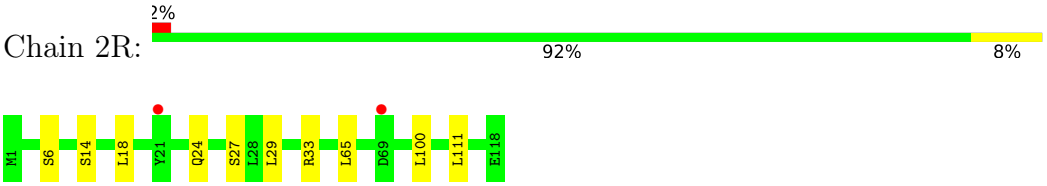




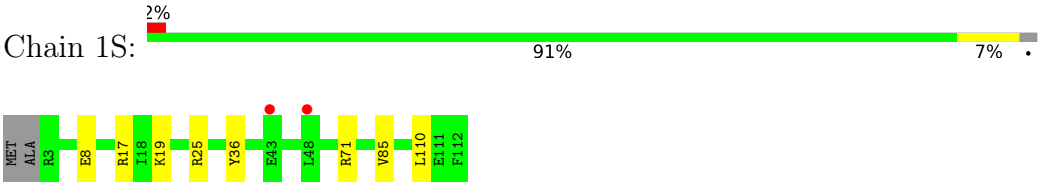
• Molecule 13: 50S ribosomal protein L17



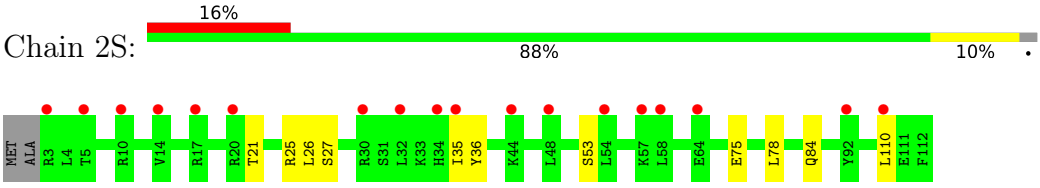
• Molecule 13: 50S ribosomal protein L17



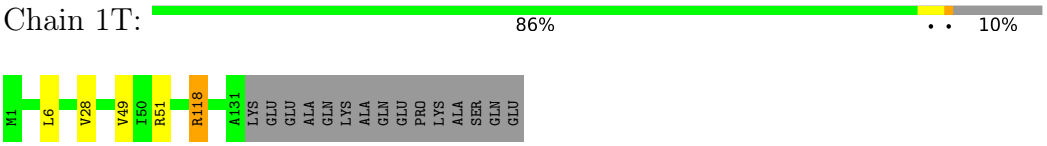
• Molecule 14: 50S ribosomal protein L18



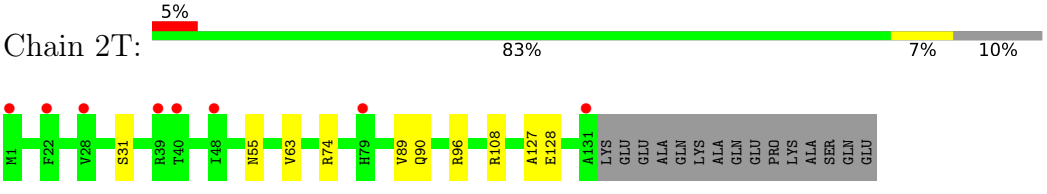
• Molecule 14: 50S ribosomal protein L18



• Molecule 15: 50S ribosomal protein L19

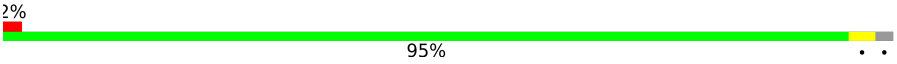


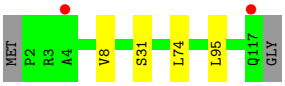
• Molecule 15: 50S ribosomal protein L19



• Molecule 16: 50S ribosomal protein L20

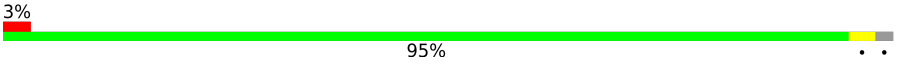
Chain 1U:





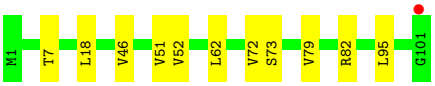
• Molecule 16: 50S ribosomal protein L20

Chain 2U:



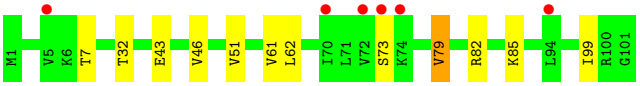
• Molecule 17: 50S ribosomal protein L21

Chain 1V:



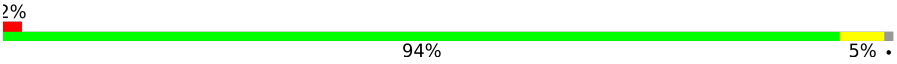
• Molecule 17: 50S ribosomal protein L21

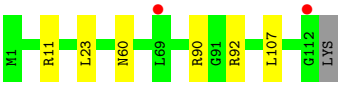
Chain 2V:



• Molecule 18: 50S ribosomal protein L22

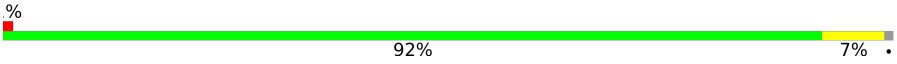
Chain 1W:

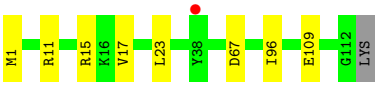




• Molecule 18: 50S ribosomal protein L22

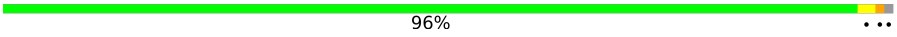
Chain 2W:

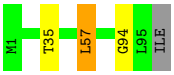




• Molecule 19: 50S ribosomal protein L23

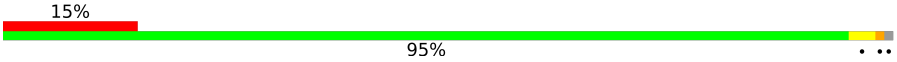
Chain 1X:

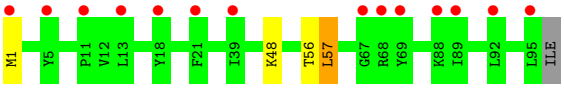




• Molecule 19: 50S ribosomal protein L23

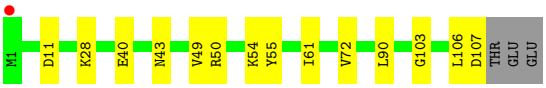
Chain 2X:





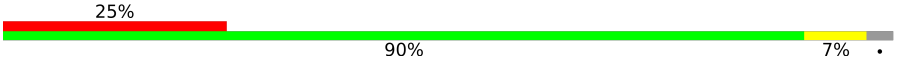
• Molecule 20: 50S ribosomal protein L24

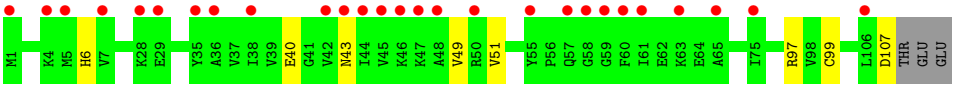
Chain 1Y:



• Molecule 20: 50S ribosomal protein L24

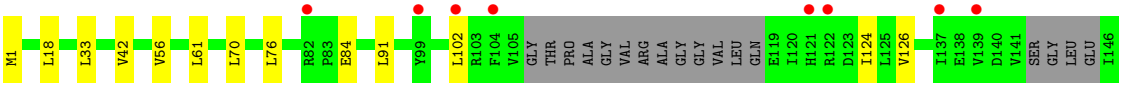
Chain 2Y:

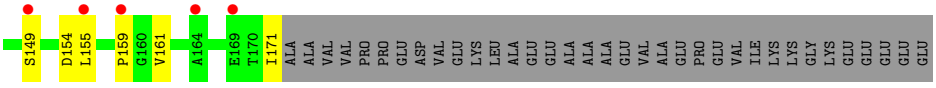




• Molecule 21: 50S ribosomal protein L25

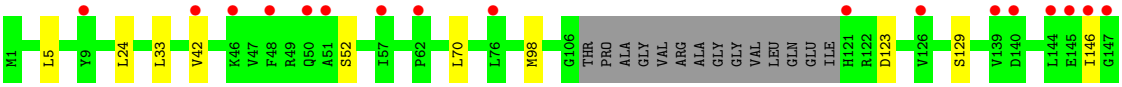
Chain 1Z:

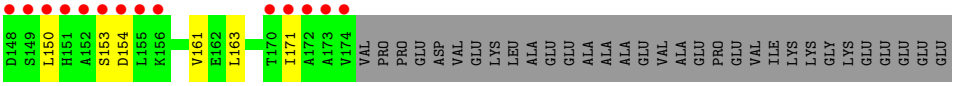




• Molecule 21: 50S ribosomal protein L25

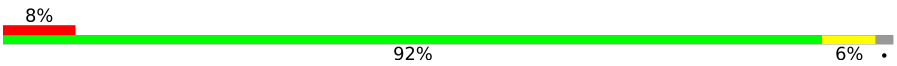
Chain 2Z:



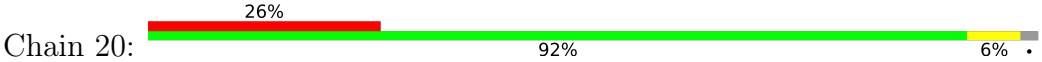


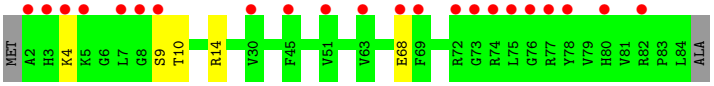
• Molecule 22: 50S ribosomal protein L27

Chain 10:

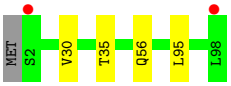


• Molecule 22: 50S ribosomal protein L27

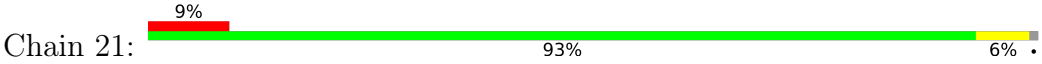


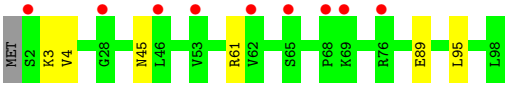


• Molecule 23: 50S ribosomal protein L28

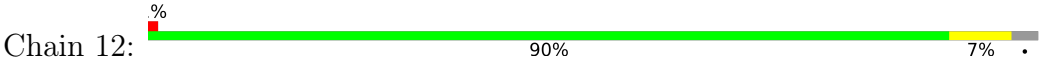


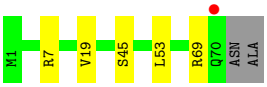
• Molecule 23: 50S ribosomal protein L28



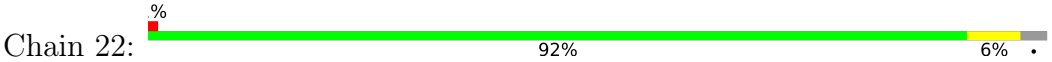


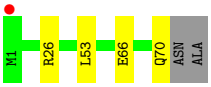
• Molecule 24: 50S ribosomal protein L29



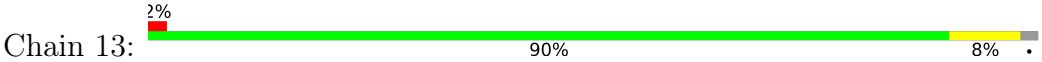


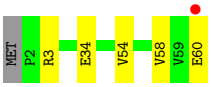
• Molecule 24: 50S ribosomal protein L29





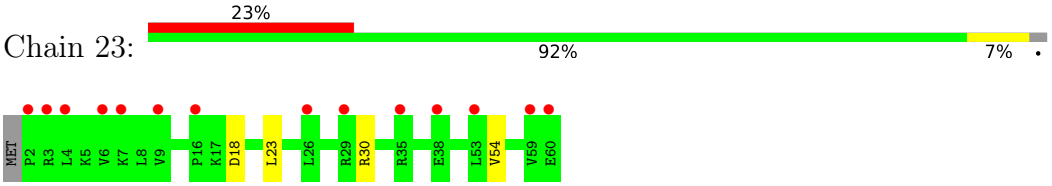
• Molecule 25: 50S ribosomal protein L30





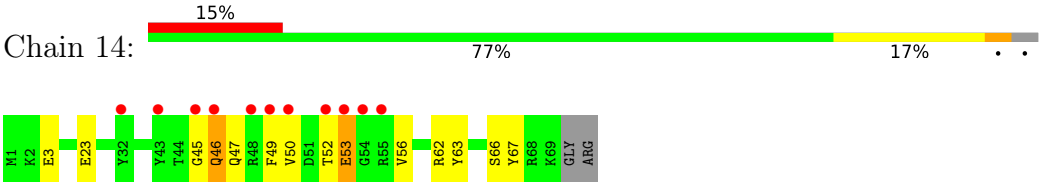
• Molecule 25: 50S ribosomal protein L30

Chain 23:



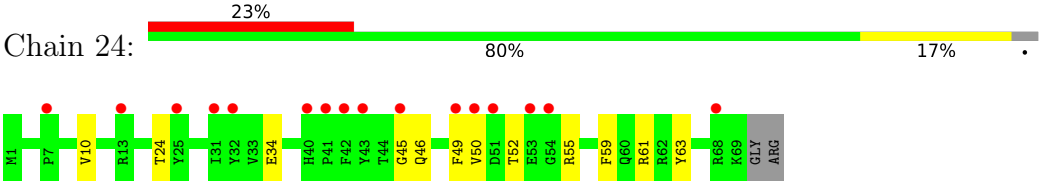
• Molecule 26: 50S ribosomal protein L31

Chain 14:



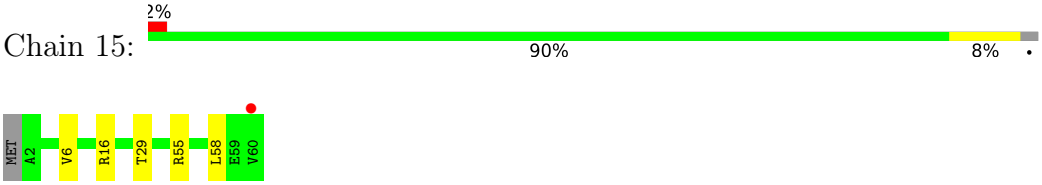
• Molecule 26: 50S ribosomal protein L31

Chain 24:



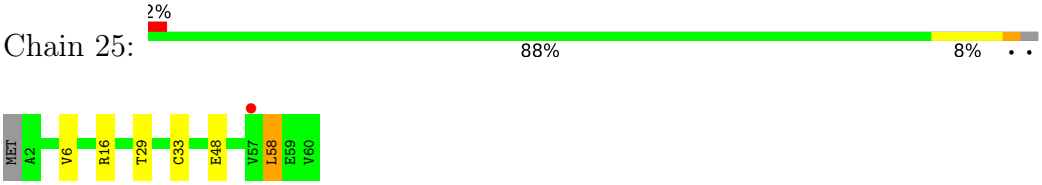
• Molecule 27: 50S ribosomal protein L32

Chain 15:



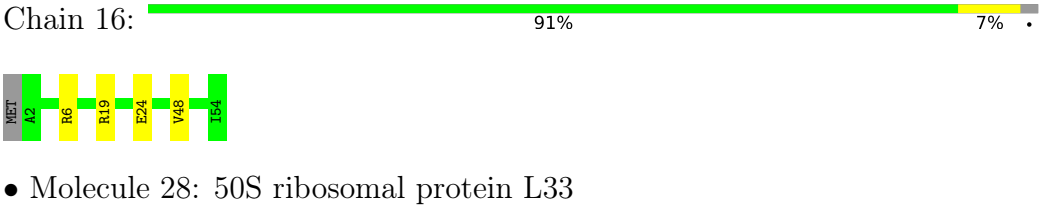
• Molecule 27: 50S ribosomal protein L32

Chain 25:



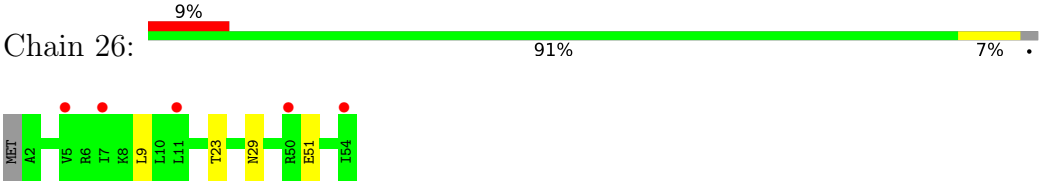
• Molecule 28: 50S ribosomal protein L33

Chain 16:



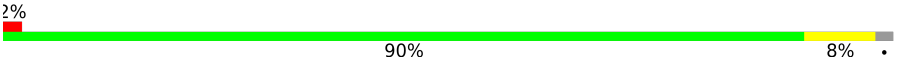
• Molecule 28: 50S ribosomal protein L33

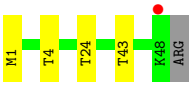
Chain 26:



• Molecule 29: 50S ribosomal protein L34

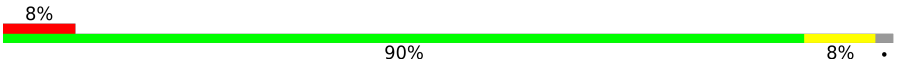
Chain 17:

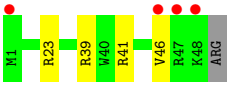




• Molecule 29: 50S ribosomal protein L34

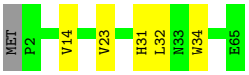
Chain 27:





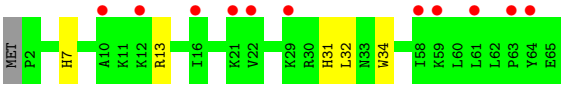
• Molecule 30: 50S ribosomal protein L35

Chain 18:



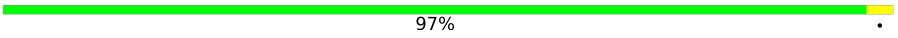
• Molecule 30: 50S ribosomal protein L35

Chain 28:



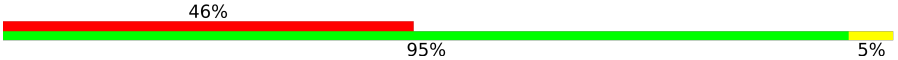
• Molecule 31: 50S ribosomal protein L36

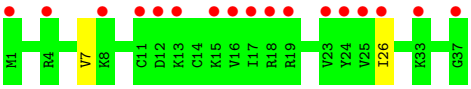
Chain 19:



• Molecule 31: 50S ribosomal protein L36

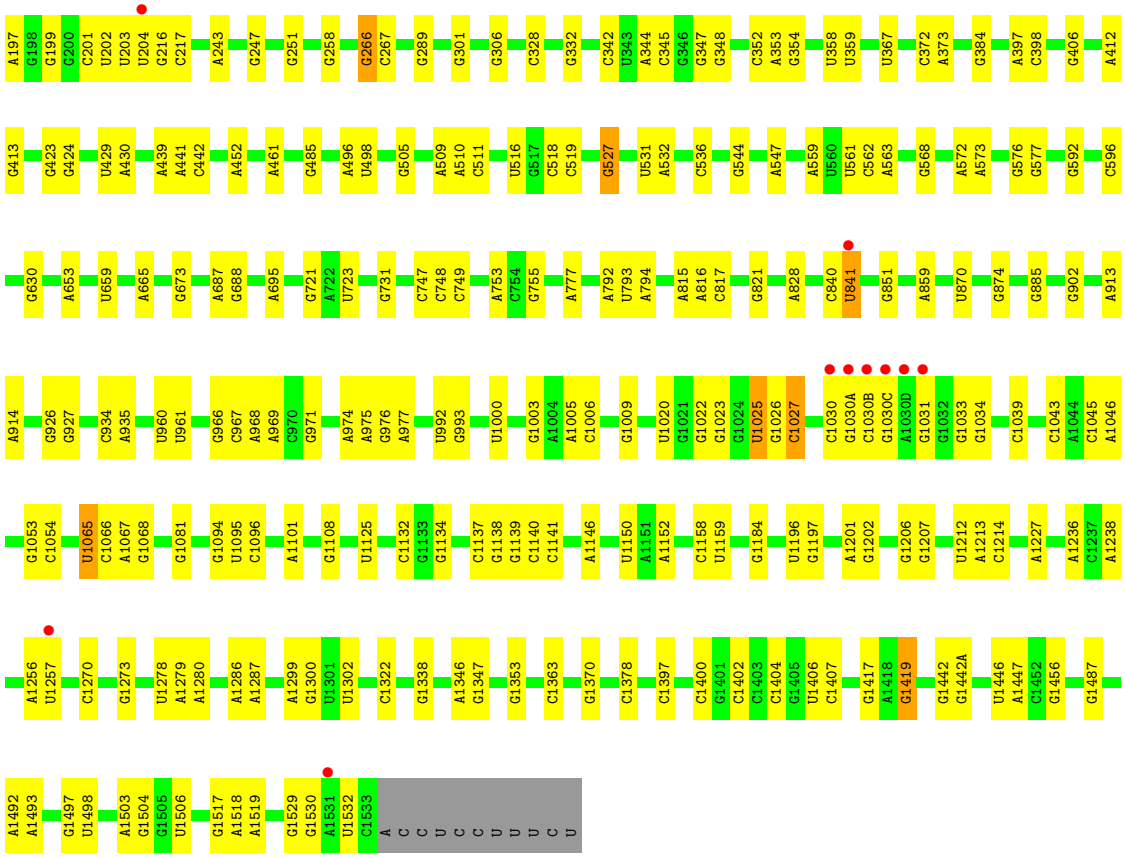
Chain 29:





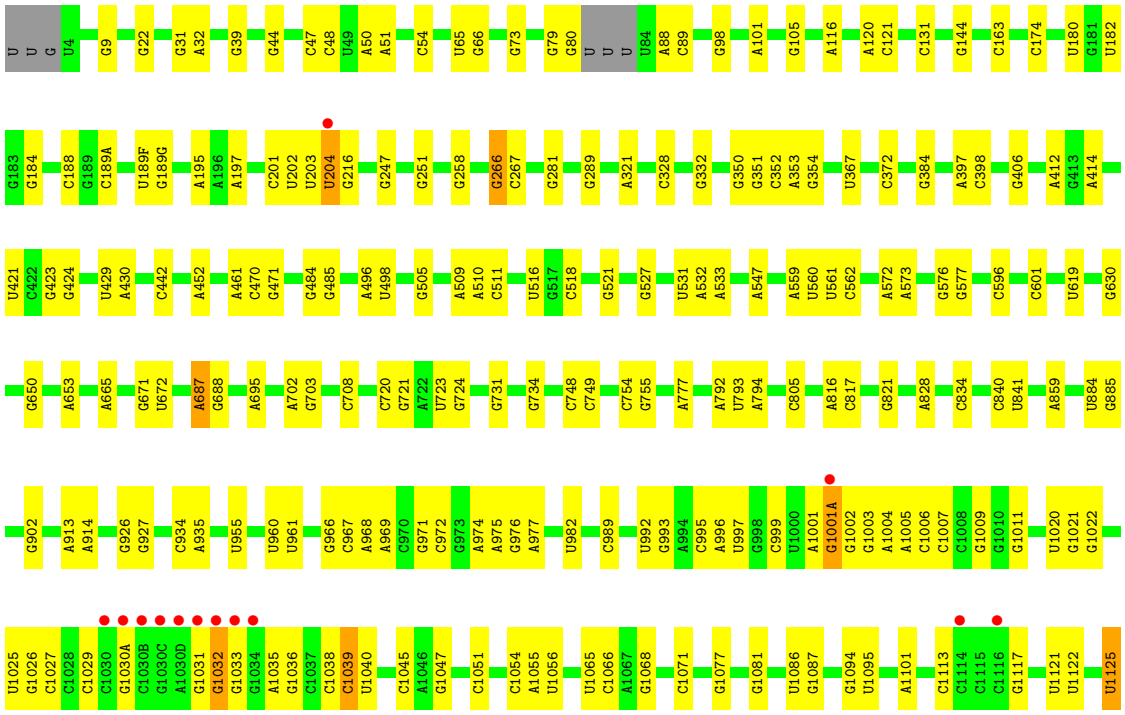
• Molecule 32: 16S Ribosomal RNA

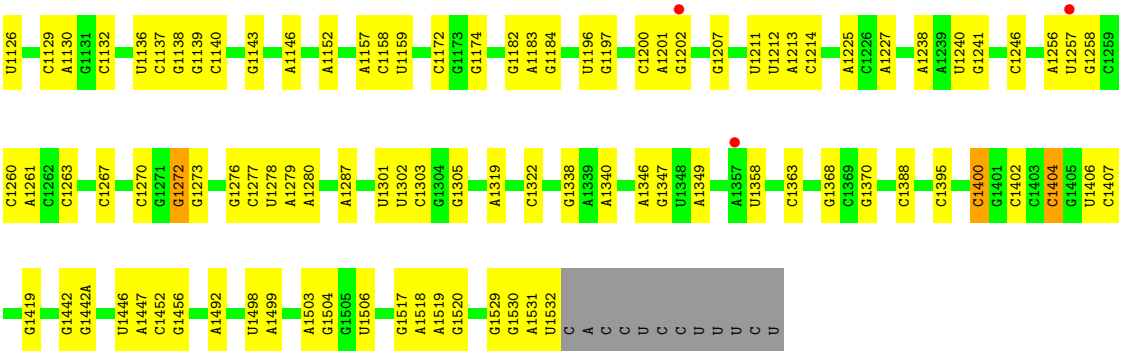
Chain 1a:



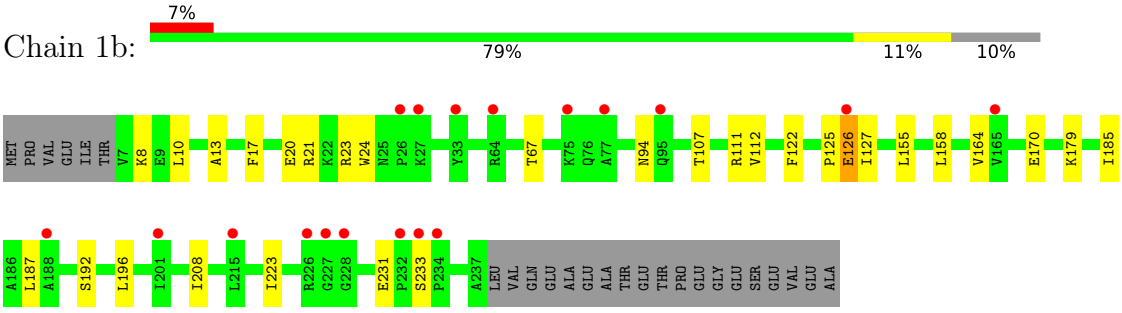
• Molecule 32: 16S Ribosomal RNA

Chain 2a:

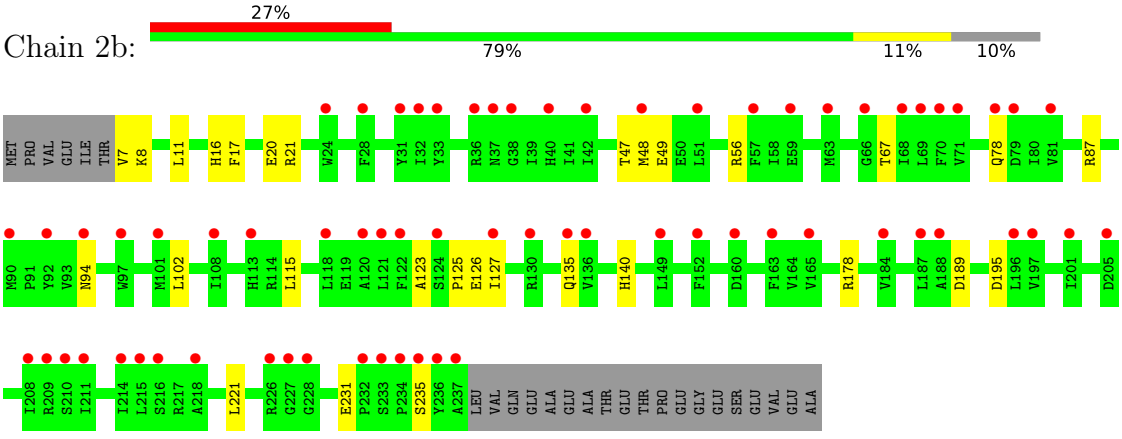




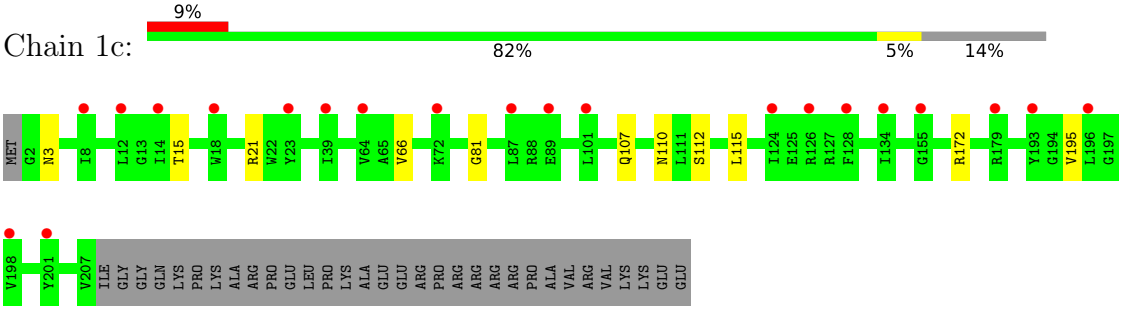
• Molecule 33: 30S ribosomal protein S2



• Molecule 33: 30S ribosomal protein S2

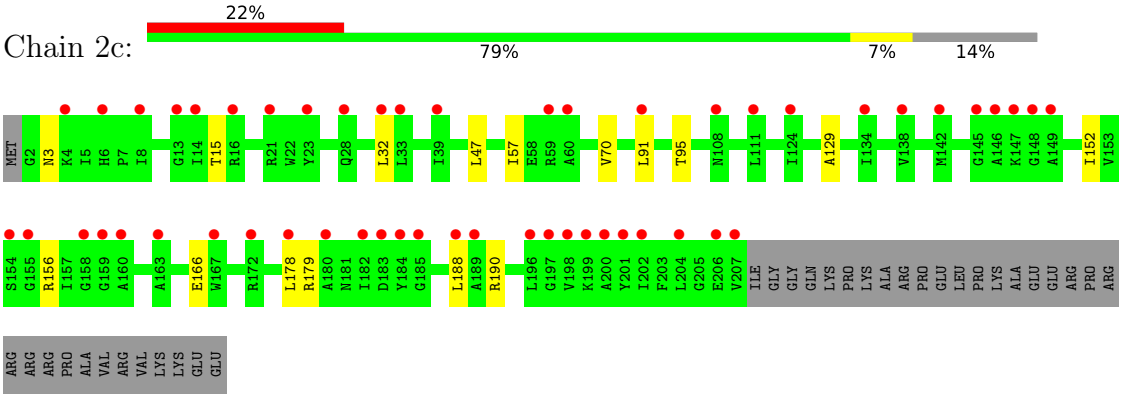


• Molecule 34: 30S ribosomal protein S3



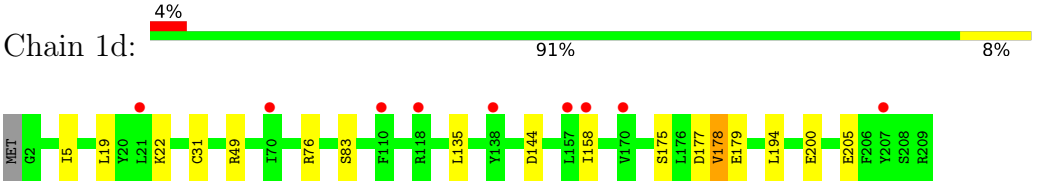
• Molecule 34: 30S ribosomal protein S3

Chain 2c:



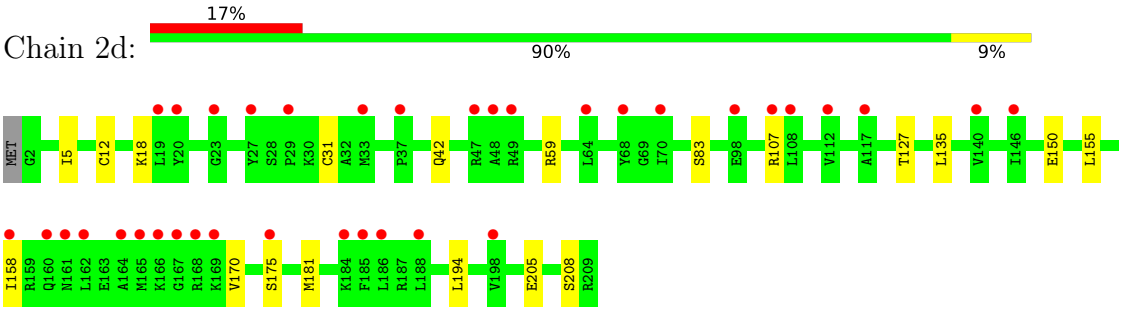
• Molecule 35: 30S ribosomal protein S4

Chain 1d:



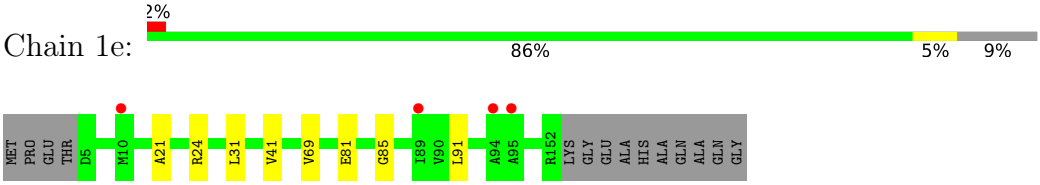
• Molecule 35: 30S ribosomal protein S4

Chain 2d:



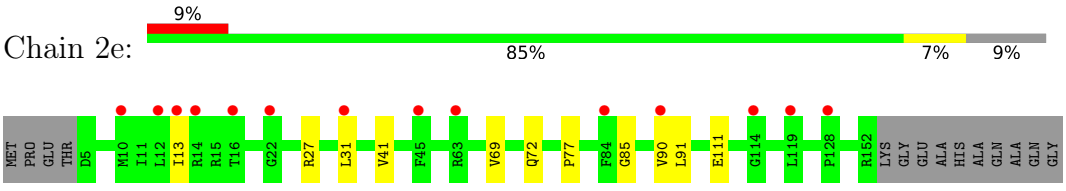
• Molecule 36: 30S ribosomal protein S5

Chain 1e:



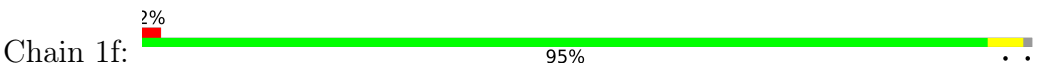
• Molecule 36: 30S ribosomal protein S5

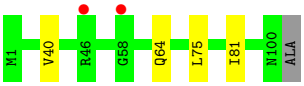
Chain 2e:



• Molecule 37: 30S ribosomal protein S6

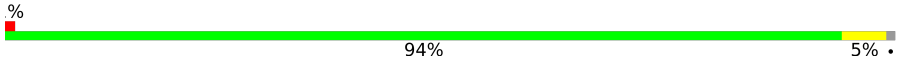
Chain 1f:

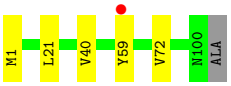




• Molecule 37: 30S ribosomal protein S6

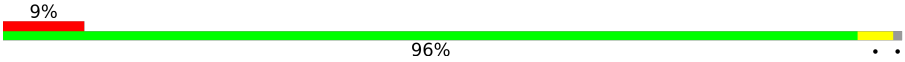
Chain 2f:

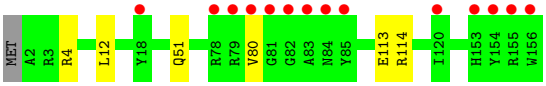




• Molecule 38: 30S ribosomal protein S7

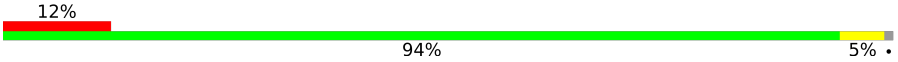
Chain 1g:





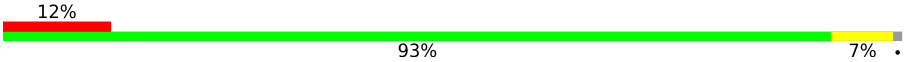
• Molecule 38: 30S ribosomal protein S7

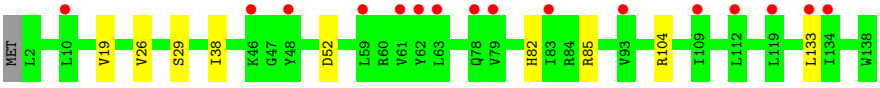
Chain 2g:



• Molecule 39: 30S ribosomal protein S8

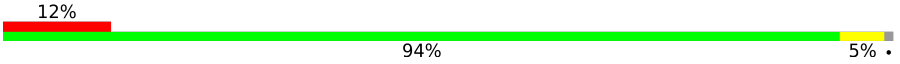
Chain 1h:

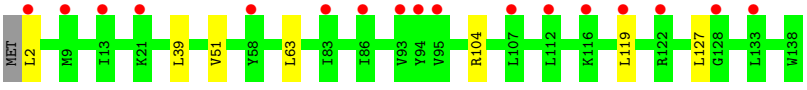




• Molecule 39: 30S ribosomal protein S8

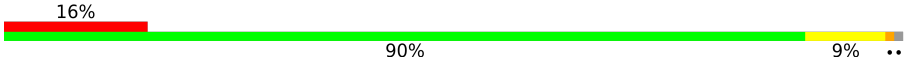
Chain 2h:

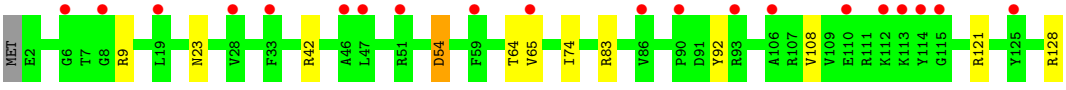




• Molecule 40: 30S ribosomal protein S9

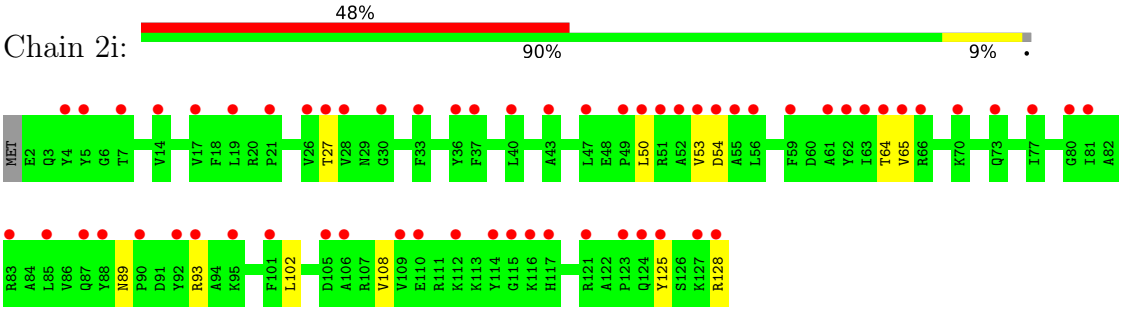
Chain 1i:





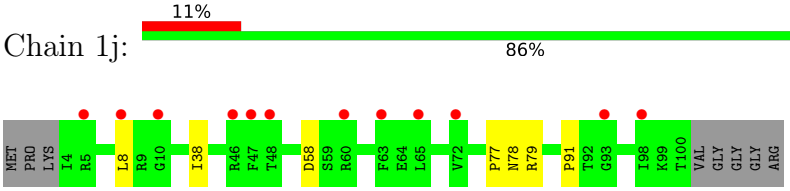
• Molecule 40: 30S ribosomal protein S9

Chain 2i:



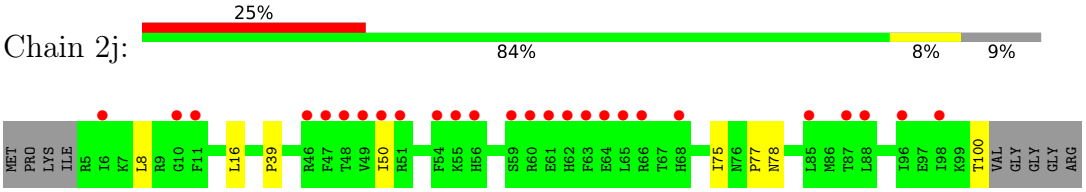
• Molecule 41: 30S ribosomal protein S10

Chain 1j:



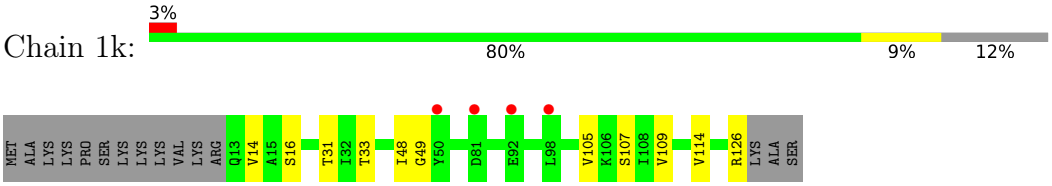
• Molecule 41: 30S ribosomal protein S10

Chain 2j:



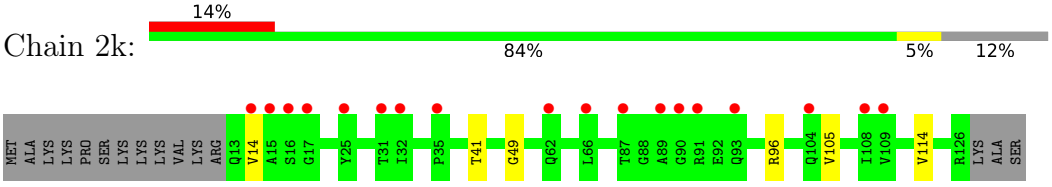
• Molecule 42: 30S ribosomal protein S11

Chain 1k:



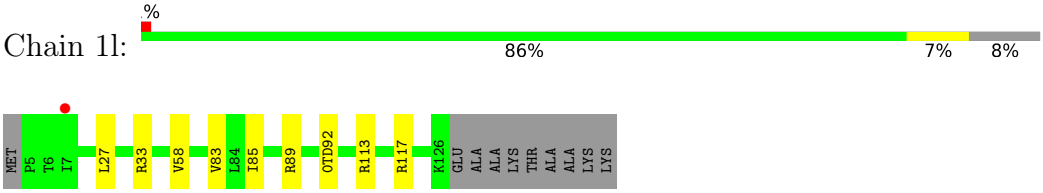
• Molecule 42: 30S ribosomal protein S11

Chain 2k:



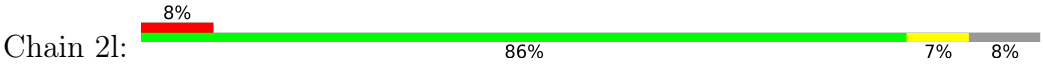
• Molecule 43: 30S ribosomal protein S12

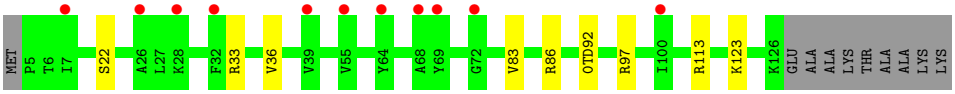
Chain 1l:



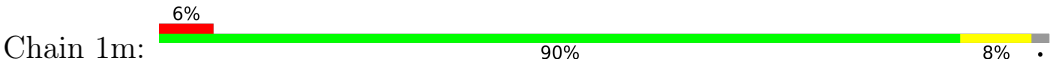
• Molecule 43: 30S ribosomal protein S12

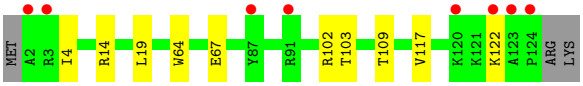
Chain 2l:



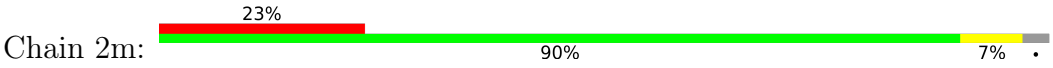


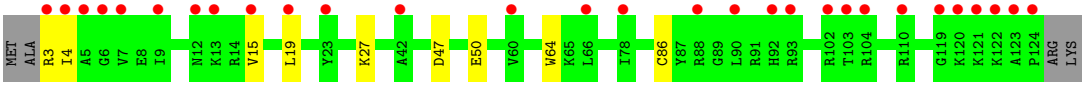
• Molecule 44: 30S ribosomal protein S13



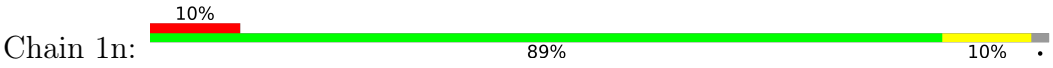


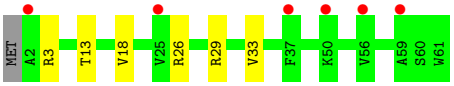
• Molecule 44: 30S ribosomal protein S13



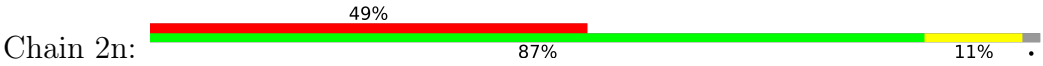


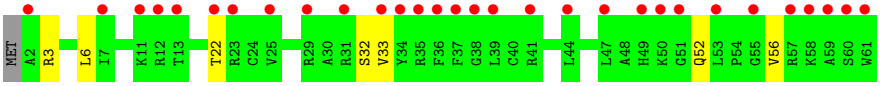
• Molecule 45: 30S ribosomal protein S14 type Z



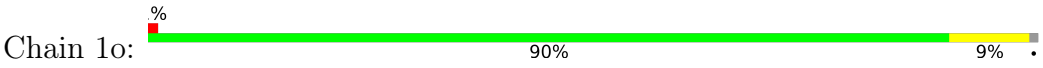


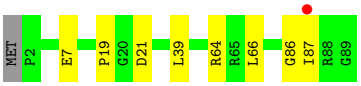
• Molecule 45: 30S ribosomal protein S14 type Z



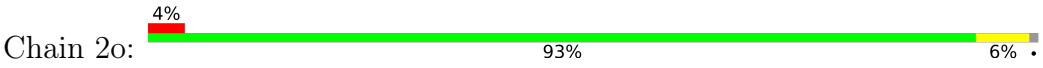


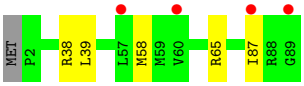
• Molecule 46: 30S ribosomal protein S15





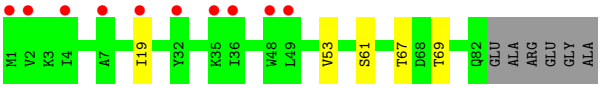
• Molecule 46: 30S ribosomal protein S15





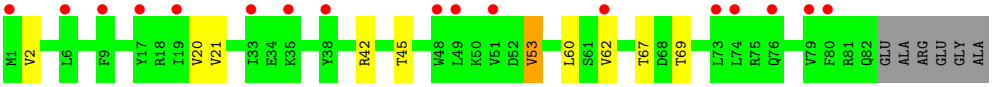
• Molecule 47: 30S ribosomal protein S16

Chain 1p:



• Molecule 47: 30S ribosomal protein S16

Chain 2p:

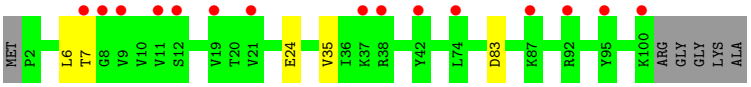


• Molecule 48: 30S ribosomal protein S17

Chain 1q:

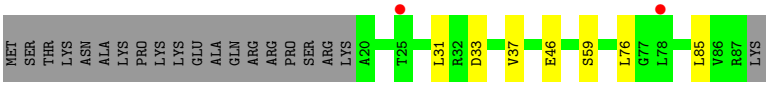
• Molecule 48: 30S ribosomal protein S17

Chain 2q:



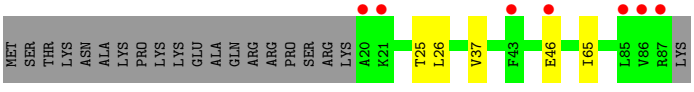
• Molecule 49: 30S ribosomal protein S18

Chain 1r:



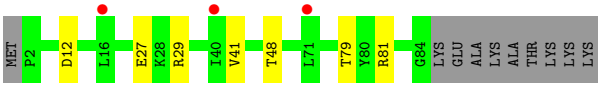
• Molecule 49: 30S ribosomal protein S18

Chain 2r:



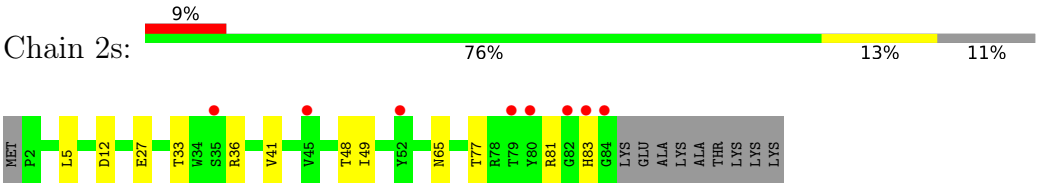
• Molecule 50: 30S ribosomal protein S19

Chain 1s:



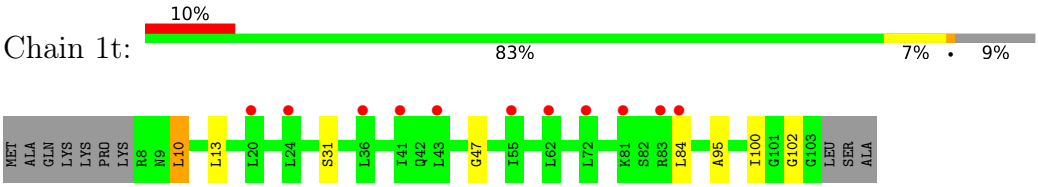
• Molecule 50: 30S ribosomal protein S19

Chain 2s:



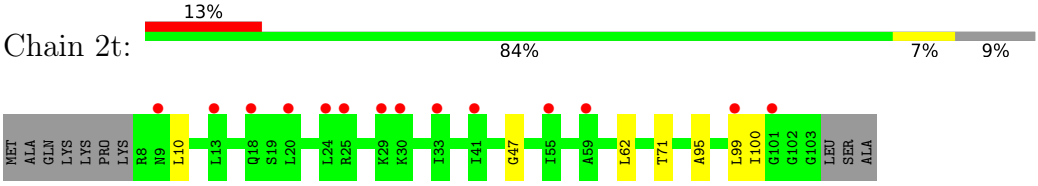
• Molecule 51: 30S ribosomal protein S20

Chain 1t:



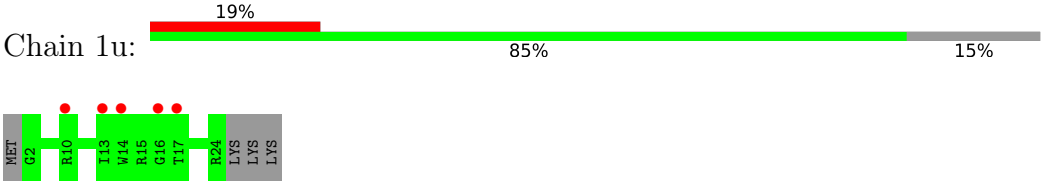
• Molecule 51: 30S ribosomal protein S20

Chain 2t:



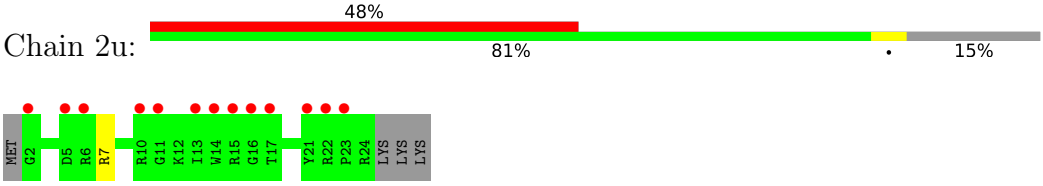
• Molecule 52: 30S ribosomal protein Thx

Chain 1u:



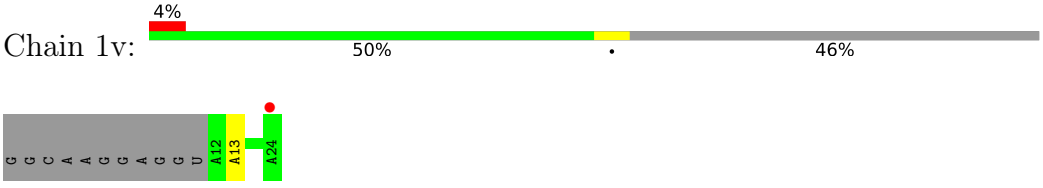
• Molecule 52: 30S ribosomal protein Thx

Chain 2u:



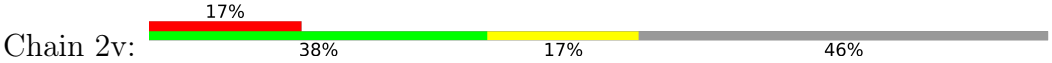
• Molecule 53: mRNA

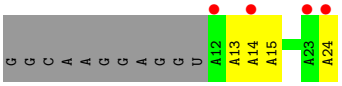
Chain 1v:



• Molecule 53: mRNA

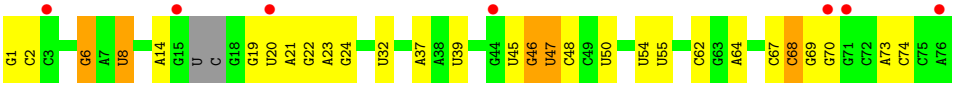
Chain 2v:





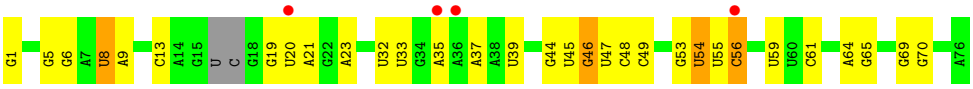
• Molecule 54: A-site and E-site tRNAs

Chain 1w:



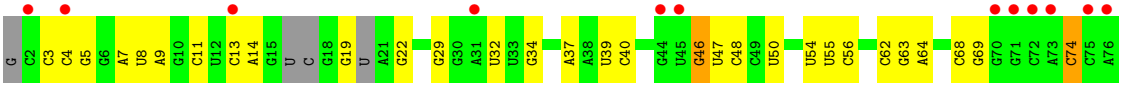
• Molecule 54: A-site and E-site tRNAs

Chain 1y:



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

Chain 2w:

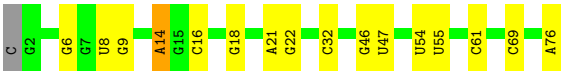


• Molecule 54: A-site and E-site tRNAs

Chain 2y:

• Molecule 55: P-site tRNA

Chain 1x:



• Molecule 55: P-site tRNA

Chain 2x:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	209.36Å 447.53Å 617.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	152.88 – 2.89 152.88 – 2.89	Depositor EDS
% Data completeness (in resolution range)	98.5 (152.88-2.89) 98.5 (152.88-2.89)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.11 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.216 , 0.263 0.216 , 0.263	Depositor DCC
R_{free} test set	63210 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	69.3	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 60.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	297628	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.46% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: SF4, 7MG, UR3, 5MU, 2MU, 2MA, OMG, MA6, KAN, 2MG, PSU, MG, MIA, 5MC, ZN, 4SU, M2G, 0TD, 4OC

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	0.51	0/69009	0.93	49/107712 (0.0%)
1	2A	0.39	0/67293	0.87	40/105034 (0.0%)
2	1B	0.44	1/2882 (0.0%)	0.87	0/4494
2	2B	0.41	1/2879 (0.0%)	0.87	2/4487 (0.0%)
3	1D	0.36	0/2186	0.54	0/2944
3	2D	0.32	0/2186	0.53	0/2944
4	1E	0.34	0/1592	0.55	0/2149
4	2E	0.31	0/1592	0.50	0/2149
5	1F	0.33	0/1619	0.51	0/2193
5	2F	0.30	0/1615	0.49	0/2188
6	1G	0.31	0/1448	0.52	0/1957
6	2G	0.34	0/1453	0.53	1/1963 (0.1%)
7	1H	0.34	0/1356	0.50	0/1834
7	2H	0.29	0/1356	0.47	0/1834
8	1I	0.28	0/1112	0.49	0/1514
8	2I	0.28	0/1079	0.49	0/1475
9	1N	0.33	0/1144	0.49	0/1543
9	2N	0.28	0/1144	0.47	0/1543
10	1O	0.35	0/943	0.53	0/1269
10	2O	0.33	0/943	0.52	0/1269
11	1P	0.33	0/1152	0.56	0/1533
11	2P	0.32	0/1152	0.54	0/1533
12	1Q	0.35	0/1143	0.52	0/1527
12	2Q	0.31	0/1143	0.48	0/1527
13	1R	0.30	0/982	0.54	0/1312
13	2R	0.28	0/982	0.52	0/1312
14	1S	0.31	0/883	0.49	0/1176
14	2S	0.31	0/880	0.50	0/1172
15	1T	0.31	0/1105	0.52	0/1477
15	2T	0.30	0/1097	0.49	0/1468
16	1U	0.35	0/977	0.49	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	2U	0.29	0/977	0.43	0/1301
17	1V	0.34	0/782	0.55	0/1049
17	2V	0.30	0/782	0.53	0/1049
18	1W	0.35	0/897	0.50	0/1205
18	2W	0.29	0/897	0.47	0/1205
19	1X	0.37	0/764	0.55	1/1025 (0.1%)
19	2X	0.28	0/764	0.56	1/1025 (0.1%)
20	1Y	0.33	0/819	0.51	0/1095
20	2Y	0.30	0/819	0.49	0/1095
21	1Z	0.31	0/1267	0.53	0/1717
21	2Z	0.30	0/1299	0.48	0/1763
22	10	0.36	0/662	0.56	1/881 (0.1%)
22	20	0.32	0/662	0.48	0/881
23	11	0.35	0/762	0.52	0/1014
23	21	0.31	0/762	0.50	0/1014
24	12	0.36	0/590	0.56	1/781 (0.1%)
24	22	0.28	0/590	0.41	0/781
25	13	0.37	0/474	0.50	0/635
25	23	0.28	0/469	0.46	0/630
26	14	0.31	0/565	0.58	0/761
26	24	0.35	0/545	0.55	0/737
27	15	0.34	0/469	0.52	0/635
27	25	0.31	0/469	0.55	1/635 (0.2%)
28	16	0.34	0/460	0.52	0/613
28	26	0.31	0/456	0.52	0/608
29	17	0.33	0/426	0.50	0/561
29	27	0.30	0/426	0.54	0/561
30	18	0.31	0/525	0.52	0/691
30	28	0.29	0/525	0.47	0/691
31	19	0.35	0/310	0.55	0/407
31	29	0.28	0/310	0.52	0/407
32	1a	0.38	0/35795	0.91	41/55864 (0.1%)
32	2a	0.36	3/35886 (0.0%)	0.89	48/56005 (0.1%)
33	1b	0.30	0/1881	0.49	0/2542
33	2b	0.30	0/1860	0.49	0/2518
34	1c	0.28	0/1572	0.48	0/2126
34	2c	0.30	0/1566	0.48	0/2119
35	1d	0.29	0/1685	0.47	0/2262
35	2d	0.28	0/1704	0.46	0/2284
36	1e	0.31	0/1145	0.52	0/1543
36	2e	0.30	0/1149	0.52	0/1548
37	1f	0.30	0/823	0.49	0/1115
37	2f	0.29	0/829	0.46	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	1g	0.28	0/1250	0.44	0/1679
38	2g	0.28	0/1254	0.43	0/1683
39	1h	0.29	0/1108	0.49	0/1494
39	2h	0.29	0/1108	0.48	0/1494
40	1i	0.29	0/1002	0.52	0/1346
40	2i	0.30	0/997	0.52	0/1343
41	1j	0.29	0/722	0.48	0/982
41	2j	0.32	0/727	0.51	0/988
42	1k	0.30	0/844	0.50	0/1145
42	2k	0.31	0/848	0.49	0/1149
43	1l	0.31	0/937	0.52	0/1260
43	2l	0.29	0/937	0.52	0/1260
44	1m	0.28	0/969	0.48	0/1302
44	2m	0.28	0/961	0.50	0/1291
45	1n	0.30	0/501	0.46	0/664
45	2n	0.33	0/501	0.50	0/664
46	1o	0.27	0/739	0.44	0/985
46	2o	0.27	0/739	0.41	0/985
47	1p	0.28	0/697	0.50	0/939
47	2p	0.27	0/693	0.49	0/935
48	1q	0.29	0/836	0.49	0/1117
48	2q	0.29	0/836	0.46	0/1117
49	1r	0.28	0/560	0.48	0/746
49	2r	0.30	0/560	0.46	0/746
50	1s	0.28	0/667	0.52	0/900
50	2s	0.29	0/661	0.54	0/893
51	1t	0.29	0/730	0.46	0/965
51	2t	0.28	0/729	0.44	0/965
52	1u	0.27	0/203	0.49	0/266
52	2u	0.33	0/203	0.57	0/266
53	1v	0.36	0/310	0.86	0/480
53	2v	0.52	0/310	0.86	0/480
54	1w	0.53	1/1606 (0.1%)	1.13	7/2497 (0.3%)
54	1y	0.57	1/1606 (0.1%)	1.13	10/2497 (0.4%)
54	2w	0.47	0/1556	1.11	1/2418 (0.0%)
54	2y	0.60	1/1583 (0.1%)	1.17	4/2459 (0.2%)
55	1x	0.52	1/1725 (0.1%)	1.11	14/2689 (0.5%)
55	2x	0.48	0/1725	1.09	9/2689 (0.3%)
All	All	0.40	9/316686 (0.0%)	0.82	231/474113 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
33	1b	0	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	1	G	OP3-P	-10.31	1.48	1.61
54	2y	1	G	OP3-P	-10.21	1.49	1.61
54	1y	1	G	OP3-P	-10.17	1.49	1.61
2	1B	1	U	OP3-P	-10.14	1.49	1.61
2	2B	1	U	OP3-P	-10.14	1.49	1.61
32	2a	1272	G	N1-C2	-8.40	1.31	1.37
32	2a	1272	G	C6-N1	-7.76	1.34	1.39
55	1x	22	G	N7-C5	5.33	1.42	1.39
32	2a	1263	C	N3-C4	-5.13	1.30	1.33

All (231) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	1a	359	U	O5'-P-OP1	-30.10	74.58	110.70
32	1a	359	U	OP1-P-OP2	-28.22	77.28	119.60
32	2a	1263	C	N1-C2-O2	20.29	131.07	118.90
32	2a	1272	G	N3-C2-N2	19.16	133.31	119.90
32	1a	359	U	O5'-P-OP2	17.44	131.63	110.70
32	2a	1272	G	N1-C2-N2	-17.01	100.89	116.20
32	2a	1272	G	C5-C6-O6	16.39	138.44	128.60
32	2a	1263	C	C2-N3-C4	14.64	127.22	119.90
1	1A	1121	C	N1-C2-O2	13.66	127.09	118.90
32	1a	358	U	OP1-P-O3'	13.22	134.28	105.20
32	1a	358	U	OP2-P-O3'	-13.09	76.39	105.20
1	1A	1109	G	C5-C6-O6	12.26	135.96	128.60
32	2a	1272	G	C6-N1-C2	11.36	131.92	125.10
1	1A	1121	C	C2-N3-C4	11.08	125.44	119.90
32	2a	1263	C	N3-C2-O2	-10.98	114.22	121.90
32	2a	1263	C	C5-C6-N1	10.87	126.43	121.00
2	2B	80	U	O4'-C1'-N1	10.74	116.80	108.20
32	2a	1272	G	C5-C6-N1	-10.61	106.20	111.50
1	1A	1132	A	N1-C6-N6	-10.26	112.45	118.60
32	1a	1027	C	C5-C4-N4	10.06	127.24	120.20
32	1a	1027	C	N3-C2-O2	-9.82	115.02	121.90
55	1x	46	G	C6-N1-C2	-9.68	119.29	125.10
1	2A	2136	C	N1-C2-O2	9.37	124.52	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	1109	G	C6-N1-C2	9.22	130.63	125.10
32	2a	1272	G	C2-N3-C4	-8.64	107.58	111.90
32	2a	1263	C	C6-N1-C2	-8.52	116.89	120.30
32	1a	1034	G	N9-C4-C5	-8.39	102.04	105.40
6	2G	43	LEU	CB-CG-CD1	8.34	125.17	111.00
1	1A	1109	G	N3-C2-N2	8.32	125.73	119.90
54	1y	33	U	C2-N1-C1'	8.19	127.53	117.70
1	2A	2473	U	C2-N1-C1'	7.96	127.25	117.70
32	1a	1034	G	N3-C2-N2	7.87	125.41	119.90
1	1A	1121	C	N3-C2-O2	-7.84	116.41	121.90
24	12	7	ARG	NE-CZ-NH2	7.78	124.19	120.30
55	2x	46	G	C6-N1-C2	-7.76	120.44	125.10
32	1a	1027	C	N3-C4-C5	-7.69	118.83	121.90
19	2X	57	LEU	CA-CB-CG	7.65	132.89	115.30
55	1x	22	G	N1-C6-O6	-7.62	115.33	119.90
32	2a	1272	G	N1-C6-O6	-7.59	115.34	119.90
1	1A	537	G	O4'-C1'-N9	7.56	114.25	108.20
32	2a	1263	C	C2-N1-C1'	7.55	127.11	118.80
32	2a	1001(A)	G	N3-C4-N9	7.51	130.51	126.00
55	1x	14	A	C5-N7-C8	7.49	107.64	103.90
32	1a	1027	C	C6-N1-C2	-7.46	117.32	120.30
32	2a	1263	C	C5-C4-N4	7.42	125.40	120.20
54	1w	47	U	C2-N1-C1'	7.33	126.50	117.70
1	1A	1109	G	N1-C6-O6	-7.31	115.52	119.90
54	1y	56	C	N1-C2-O2	7.29	123.28	118.90
1	1A	12	U	C2-N1-C1'	7.28	126.43	117.70
1	1A	572	A	P-O3'-C3'	7.25	128.40	119.70
1	1A	2189	U	C2-N1-C1'	7.18	126.32	117.70
32	1a	1034	G	C4-C5-N7	7.02	113.61	110.80
54	1y	33	U	N1-C2-O2	6.98	127.69	122.80
1	1A	1121	C	C5-C4-N4	6.96	125.07	120.20
32	2a	1272	G	C4-N9-C1'	6.96	135.55	126.50
32	1a	1030(B)	C	C2-N1-C1'	6.94	126.44	118.80
55	1x	22	G	C5-N7-C8	-6.94	100.83	104.30
32	2a	1272	G	C8-N9-C1'	-6.92	118.00	127.00
55	1x	22	G	C4-C5-C6	-6.91	114.65	118.80
55	1x	14	A	C4-C5-C6	6.87	120.43	117.00
1	2A	2139	C	C2-N1-C1'	6.81	126.29	118.80
32	2a	1263	C	C4-C5-C6	-6.81	114.00	117.40
54	1w	22	G	N1-C6-O6	6.76	123.95	119.90
32	1a	1027	C	C6-N1-C1'	6.64	128.77	120.80
55	2x	14	A	C4-C5-C6	6.64	120.32	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2A	2136	C	N3-C2-O2	-6.59	117.29	121.90
1	1A	2442	A	C2-N3-C4	6.56	113.88	110.60
55	2x	22	G	N1-C6-O6	-6.55	115.97	119.90
1	2A	2897	U	C2-N1-C1'	6.50	125.50	117.70
1	1A	572	A	OP1-P-O3'	6.50	119.49	105.20
32	2a	754	C	C2-N1-C1'	6.49	125.94	118.80
32	2a	1263	C	N1-C2-N3	-6.47	114.67	119.20
32	2a	1032	G	C5-C6-O6	6.45	132.47	128.60
32	1a	1030(B)	C	N1-C2-O2	6.38	122.73	118.90
55	2x	14	A	C5-N7-C8	6.36	107.08	103.90
32	1a	1027	C	N1-C2-O2	6.35	122.71	118.90
1	1A	2189	U	N3-C2-O2	-6.35	117.76	122.20
32	1a	841	U	C5-C6-N1	6.34	125.87	122.70
55	2x	22	G	C4-C5-C6	-6.34	115.00	118.80
54	1y	64	A	C5-C6-N6	6.32	128.76	123.70
1	2A	2206	G	C4-N9-C1'	-6.30	118.31	126.50
32	1a	1034	G	N3-C4-N9	6.27	129.76	126.00
1	1A	2189	U	N1-C2-O2	6.25	127.17	122.80
32	1a	1025	U	N1-C2-O2	6.24	127.17	122.80
55	1x	46	G	N3-C2-N2	-6.23	115.54	119.90
54	1y	64	A	N1-C6-N6	-6.19	114.88	118.60
1	2A	1313	U	C2-N1-C1'	6.19	125.13	117.70
1	1A	2180	A	P-O3'-C3'	6.18	127.11	119.70
32	1a	1417	G	N3-C2-N2	6.18	124.22	119.90
54	1w	47	U	N1-C2-O2	6.17	127.12	122.80
1	1A	2485	U	N3-C2-O2	-6.13	117.91	122.20
54	2y	22	G	N1-C6-O6	6.12	123.57	119.90
1	1A	2331	G	O4'-C1'-N9	6.11	113.08	108.20
1	1A	894	U	C2-N1-C1'	6.09	125.01	117.70
54	2y	58	A	OP1-P-O3'	6.08	118.57	105.20
32	2a	754	C	N1-C2-O2	6.06	122.54	118.90
1	2A	2129	C	N1-C2-O2	6.04	122.52	118.90
1	2A	2447	G	C4-N9-C1'	-6.03	118.67	126.50
32	1a	266	G	P-O3'-C3'	6.02	126.93	119.70
1	1A	1221	G	OP1-P-O3'	6.00	118.40	105.20
1	1A	1109	G	C5-C6-N1	-5.96	108.52	111.50
55	1x	14	A	C5-C6-N1	-5.93	114.74	117.70
55	1x	46	G	N1-C2-N3	5.92	127.45	123.90
32	1a	1417	G	N1-C6-O6	-5.89	116.37	119.90
1	1A	2641	A	P-O3'-C3'	5.87	126.75	119.70
32	2a	1039	C	C2-N1-C1'	5.84	125.22	118.80
32	2a	1225	A	C5-C6-N6	5.83	128.36	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	1a	1027	C	N3-C4-N4	-5.81	113.93	118.00
27	25	58	LEU	CA-CB-CG	5.81	128.66	115.30
55	2x	14	A	C5-C6-N1	-5.81	114.80	117.70
1	2A	1532	C	C2-N1-C1'	5.80	125.18	118.80
1	2A	2139	C	N1-C2-O2	5.80	122.38	118.90
1	1A	399	G	O4'-C1'-N9	5.78	112.83	108.20
32	2a	79	G	C5-C6-O6	5.77	132.06	128.60
32	2a	1263	C	N3-C4-N4	-5.77	113.96	118.00
1	1A	1132	A	C5-C6-N6	5.72	128.28	123.70
32	2a	65	U	P-O3'-C3'	5.69	126.53	119.70
1	1A	2228	G	C4-N9-C1'	5.68	133.89	126.50
32	1a	1030(B)	C	C6-N1-C2	-5.68	118.03	120.30
1	2A	2140	C	C2-N1-C1'	5.68	125.05	118.80
32	2a	204	U	C2-N1-C1'	5.67	124.51	117.70
1	1A	2014	G	P-O3'-C3'	5.67	126.50	119.70
1	2A	2689	U	P-O3'-C3'	5.66	126.49	119.70
32	2a	1001(A)	G	C4-N9-C1'	5.66	133.86	126.50
1	1A	1878	A	O4'-C1'-N9	5.66	112.72	108.20
55	1x	46	G	C5-C6-N1	5.66	114.33	111.50
32	1a	1419	G	N3-C2-N2	5.64	123.85	119.90
32	2a	955	U	C2-N3-C4	5.64	130.38	127.00
32	1a	1158	C	C2-N1-C1'	5.64	125.00	118.80
54	1y	33	U	N3-C2-O2	-5.63	118.26	122.20
32	1a	1034	G	C6-N1-C2	5.61	128.47	125.10
54	1w	6	G	C5-C6-O6	-5.58	125.25	128.60
32	2a	1126	U	C2-N1-C1'	5.58	124.39	117.70
1	1A	2451	A	O4'-C1'-N9	-5.57	103.74	108.20
1	2A	228	A	OP1-P-O3'	5.57	117.45	105.20
32	2a	266	G	P-O3'-C3'	5.55	126.36	119.70
1	1A	2513	C	C2-N1-C1'	-5.51	112.74	118.80
1	2A	2473	U	N1-C2-O2	5.50	126.65	122.80
1	2A	214	G	O4'-C1'-N9	5.48	112.58	108.20
1	2A	2139	C	C6-N1-C1'	-5.48	114.22	120.80
1	1A	1128	U	N3-C4-O4	-5.47	115.57	119.40
32	1a	913	A	P-O3'-C3'	5.46	126.26	119.70
54	1w	67	C	C2-N1-C1'	5.45	124.80	118.80
1	1A	894	U	N1-C2-O2	5.45	126.61	122.80
1	1A	2485	U	N1-C2-O2	5.42	126.59	122.80
1	2A	1992	G	P-O3'-C3'	5.42	126.20	119.70
1	2A	2174	C	N1-C2-O2	5.42	122.15	118.90
54	1y	33	U	C6-N1-C1'	-5.40	113.64	121.20
32	1a	1030(B)	C	N3-C2-O2	-5.40	118.12	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	1001(A)	G	C8-N9-C1'	-5.39	119.99	127.00
1	2A	528	A	P-O3'-C3'	5.39	126.16	119.70
1	1A	1222	A	O5'-P-OP1	-5.38	100.85	105.70
1	1A	2485	U	C2-N1-C1'	5.38	124.16	117.70
32	1a	1417	G	C5-C6-O6	5.37	131.82	128.60
32	1a	90	U	N1-C2-O2	5.37	126.56	122.80
1	2A	1204	A	O4'-C1'-N9	5.36	112.49	108.20
32	1a	1158	C	N1-C2-O2	5.35	122.11	118.90
54	2y	58	A	P-O3'-C3'	5.33	126.10	119.70
54	1y	56	C	C2-N3-C4	5.33	122.56	119.90
1	2A	1698	A	O4'-C1'-N9	5.29	112.43	108.20
32	2a	1001(A)	G	N3-C4-C5	-5.29	125.96	128.60
32	1a	90	U	N3-C2-O2	-5.28	118.50	122.20
1	2A	228	A	P-O3'-C3'	5.27	126.02	119.70
1	2A	2174	C	C2-N1-C1'	5.26	124.59	118.80
32	2a	1039	C	C5-C4-N4	-5.26	116.52	120.20
32	2a	1125	U	N1-C2-O2	5.26	126.48	122.80
1	1A	1121	C	C5-C6-N1	5.26	123.63	121.00
1	2A	1653	G	P-O3'-C3'	5.26	126.01	119.70
32	1a	1025	U	N3-C2-O2	-5.26	118.52	122.20
1	2A	752	A	P-O3'-C3'	5.25	126.00	119.70
54	2w	74	C	N1-C2-O2	5.25	122.05	118.90
1	2A	2473	U	C6-N1-C1'	-5.24	113.86	121.20
1	2A	1022	G	N3-C4-N9	-5.22	122.87	126.00
32	2a	1395	C	N1-C2-O2	5.21	122.03	118.90
32	1a	1067	A	P-O3'-C3'	5.21	125.95	119.70
32	2a	1225	A	C6-N1-C2	5.20	121.72	118.60
32	1a	1065	U	P-O3'-C3'	5.20	125.94	119.70
1	2A	2473	U	N3-C2-O2	-5.20	118.56	122.20
32	2a	913	A	P-O3'-C3'	5.20	125.94	119.70
54	1w	47	U	C6-N1-C1'	-5.19	113.93	121.20
32	2a	1032	G	N1-C6-O6	-5.19	116.79	119.90
55	2x	22	G	C5-N7-C8	-5.18	101.71	104.30
32	2a	1126	U	N1-C2-O2	5.18	126.42	122.80
1	2A	847	U	C2-N1-C1'	5.17	123.91	117.70
1	1A	892	G	O4'-C1'-N9	5.17	112.34	108.20
1	2A	2206	G	C8-N9-C1'	5.17	133.72	127.00
19	1X	57	LEU	CA-CB-CG	5.16	127.16	115.30
1	2A	1460	A	O4'-C1'-N9	5.16	112.33	108.20
54	1w	68	C	C2-N1-C1'	5.15	124.46	118.80
1	2A	2629	A	O4'-C1'-N9	5.14	112.31	108.20
32	2a	1032	G	C6-N1-C2	5.14	128.19	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	1219	A	P-O3'-C3'	5.14	125.87	119.70
1	1A	410	U	C2-N1-C1'	-5.13	111.55	117.70
32	1a	1206	G	N3-C4-N9	5.13	129.08	126.00
2	2B	1	U	C2-N1-C1'	5.13	123.85	117.70
1	2A	2897	U	N1-C2-O2	5.12	126.39	122.80
1	1A	839	G	O4'-C1'-N9	-5.12	104.11	108.20
1	2A	645	C	N1-C2-O2	5.12	121.97	118.90
55	2x	22	G	C6-C5-N7	5.11	133.47	130.40
1	1A	1359	U	C2-N1-C1'	5.11	123.83	117.70
32	1a	1150	U	C2-N3-C4	5.11	130.06	127.00
54	1y	56	C	N3-C2-O2	-5.10	118.33	121.90
32	2a	1047	G	N3-C4-N9	5.10	129.06	126.00
55	1x	22	G	C5-C6-N1	5.10	114.05	111.50
1	1A	1177	G	O4'-C1'-N9	5.10	112.28	108.20
1	1A	1318	A	O5'-P-OP2	-5.09	101.12	105.70
55	1x	16	C	C4-C5-C6	5.08	119.94	117.40
1	2A	1530	C	P-O3'-C3'	5.08	125.80	119.70
32	2a	687	A	P-O3'-C3'	5.07	125.79	119.70
32	1a	748	C	P-O3'-C3'	5.06	125.77	119.70
1	2A	614	U	N3-C2-O2	-5.05	118.66	122.20
1	2A	2167	U	N3-C2-O2	-5.05	118.66	122.20
1	1A	1219	A	OP1-P-O3'	5.05	116.31	105.20
1	2A	2554	U	O5'-P-OP1	-5.05	101.16	105.70
55	1x	22	G	C8-N9-C1'	5.04	133.56	127.00
54	2y	43	C	C2-N1-C1'	5.04	124.34	118.80
1	1A	14	A	C5-C6-N1	5.04	120.22	117.70
1	2A	1992	G	C8-N9-C4	-5.04	104.39	106.40
32	1a	841	U	C6-N1-C2	-5.03	117.98	121.00
32	2a	1322	C	N1-C2-O2	-5.03	115.88	118.90
55	2x	22	G	C8-N9-C1'	5.03	133.53	127.00
54	1y	33	U	C5-C6-N1	5.03	125.21	122.70
1	1A	720	C	O5'-P-OP2	-5.02	101.18	105.70
32	2a	748	C	P-O3'-C3'	5.02	125.72	119.70
1	1A	2228	G	C8-N9-C1'	-5.02	120.47	127.00
32	1a	563	A	O4'-C1'-N9	5.02	112.22	108.20
32	2a	1225	A	N1-C6-N6	-5.02	115.59	118.60
22	10	12	ASN	C-N-CA	-5.01	111.78	122.30
1	1A	1216	G	C8-N9-C4	-5.00	104.40	106.40
55	1x	22	G	N3-C4-N9	-5.00	123.00	126.00
32	2a	1001(A)	G	C6-C5-N7	-5.00	127.40	130.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
33	1b	8	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%)	255 (93%)	18 (7%)	0	100	100
3	2D	273/276 (99%)	252 (92%)	19 (7%)	2 (1%)	22	54
4	1E	202/206 (98%)	188 (93%)	12 (6%)	2 (1%)	15	45
4	2E	202/206 (98%)	190 (94%)	10 (5%)	2 (1%)	15	45
5	1F	201/210 (96%)	195 (97%)	5 (2%)	1 (0%)	29	61
5	2F	201/210 (96%)	185 (92%)	13 (6%)	3 (2%)	10	34
6	1G	179/182 (98%)	163 (91%)	14 (8%)	2 (1%)	14	42
6	2G	179/182 (98%)	168 (94%)	10 (6%)	1 (1%)	25	58
7	1H	172/180 (96%)	163 (95%)	8 (5%)	1 (1%)	25	58
7	2H	172/180 (96%)	150 (87%)	19 (11%)	3 (2%)	9	31
8	1I	144/148 (97%)	130 (90%)	14 (10%)	0	100	100
8	2I	144/148 (97%)	121 (84%)	20 (14%)	3 (2%)	7	26
9	1N	138/140 (99%)	129 (94%)	9 (6%)	0	100	100
9	2N	138/140 (99%)	128 (93%)	8 (6%)	2 (1%)	11	36
10	1O	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
10	2O	120/122 (98%)	109 (91%)	9 (8%)	2 (2%)	9	31
11	1P	147/150 (98%)	137 (93%)	10 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
11	2P	147/150 (98%)	130 (88%)	13 (9%)	4 (3%)	5 19
12	1Q	139/141 (99%)	132 (95%)	5 (4%)	2 (1%)	11 36
12	2Q	139/141 (99%)	127 (91%)	11 (8%)	1 (1%)	22 54
13	1R	116/118 (98%)	109 (94%)	6 (5%)	1 (1%)	17 48
13	2R	116/118 (98%)	103 (89%)	12 (10%)	1 (1%)	17 48
14	1S	108/112 (96%)	102 (94%)	6 (6%)	0	100 100
14	2S	108/112 (96%)	99 (92%)	7 (6%)	2 (2%)	8 28
15	1T	129/146 (88%)	118 (92%)	10 (8%)	1 (1%)	19 51
15	2T	129/146 (88%)	120 (93%)	6 (5%)	3 (2%)	6 23
16	1U	114/118 (97%)	113 (99%)	1 (1%)	0	100 100
16	2U	114/118 (97%)	110 (96%)	4 (4%)	0	100 100
17	1V	99/101 (98%)	90 (91%)	9 (9%)	0	100 100
17	2V	99/101 (98%)	91 (92%)	7 (7%)	1 (1%)	15 45
18	1W	110/113 (97%)	108 (98%)	2 (2%)	0	100 100
18	2W	110/113 (97%)	107 (97%)	3 (3%)	0	100 100
19	1X	93/96 (97%)	89 (96%)	3 (3%)	1 (1%)	14 42
19	2X	93/96 (97%)	87 (94%)	6 (6%)	0	100 100
20	1Y	105/110 (96%)	94 (90%)	8 (8%)	3 (3%)	4 18
20	2Y	105/110 (96%)	92 (88%)	11 (10%)	2 (2%)	8 28
21	1Z	148/206 (72%)	128 (86%)	19 (13%)	1 (1%)	22 54
21	2Z	156/206 (76%)	127 (81%)	26 (17%)	3 (2%)	8 28
22	10	81/85 (95%)	80 (99%)	1 (1%)	0	100 100
22	20	81/85 (95%)	75 (93%)	5 (6%)	1 (1%)	13 40
23	11	95/98 (97%)	92 (97%)	3 (3%)	0	100 100
23	21	95/98 (97%)	92 (97%)	1 (1%)	2 (2%)	7 26
24	12	68/72 (94%)	66 (97%)	2 (3%)	0	100 100
24	22	68/72 (94%)	66 (97%)	2 (3%)	0	100 100
25	13	57/60 (95%)	54 (95%)	3 (5%)	0	100 100
25	23	57/60 (95%)	53 (93%)	4 (7%)	0	100 100
26	14	67/71 (94%)	53 (79%)	9 (13%)	5 (8%)	1 2
26	24	67/71 (94%)	52 (78%)	10 (15%)	5 (8%)	1 2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	15	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
27	25	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
28	16	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
28	26	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
29	17	46/49 (94%)	44 (96%)	2 (4%)	0	100	100
29	27	46/49 (94%)	45 (98%)	0	1 (2%)	6	24
30	18	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
30	28	62/65 (95%)	60 (97%)	1 (2%)	1 (2%)	9	32
31	19	35/37 (95%)	32 (91%)	3 (9%)	0	100	100
31	29	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
33	1b	229/256 (90%)	198 (86%)	23 (10%)	8 (4%)	3	14
33	2b	229/256 (90%)	200 (87%)	20 (9%)	9 (4%)	3	12
34	1c	204/239 (85%)	181 (89%)	20 (10%)	3 (2%)	10	34
34	2c	204/239 (85%)	172 (84%)	27 (13%)	5 (2%)	5	21
35	1d	206/209 (99%)	192 (93%)	11 (5%)	3 (2%)	10	34
35	2d	206/209 (99%)	182 (88%)	20 (10%)	4 (2%)	8	28
36	1e	146/162 (90%)	133 (91%)	10 (7%)	3 (2%)	7	26
36	2e	146/162 (90%)	131 (90%)	11 (8%)	4 (3%)	5	19
37	1f	98/101 (97%)	92 (94%)	5 (5%)	1 (1%)	15	45
37	2f	98/101 (97%)	91 (93%)	6 (6%)	1 (1%)	15	45
38	1g	153/156 (98%)	142 (93%)	9 (6%)	2 (1%)	12	37
38	2g	153/156 (98%)	137 (90%)	13 (8%)	3 (2%)	7	27
39	1h	135/138 (98%)	128 (95%)	7 (5%)	0	100	100
39	2h	135/138 (98%)	124 (92%)	11 (8%)	0	100	100
40	1i	125/128 (98%)	109 (87%)	15 (12%)	1 (1%)	19	51
40	2i	125/128 (98%)	107 (86%)	17 (14%)	1 (1%)	19	51
41	1j	95/105 (90%)	76 (80%)	15 (16%)	4 (4%)	3	10
41	2j	94/105 (90%)	79 (84%)	10 (11%)	5 (5%)	2	6
42	1k	112/129 (87%)	102 (91%)	7 (6%)	3 (3%)	5	19
42	2k	112/129 (87%)	100 (89%)	10 (9%)	2 (2%)	8	29
43	1l	119/132 (90%)	109 (92%)	10 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
43	2l	119/132 (90%)	107 (90%)	12 (10%)	0	100 100
44	1m	121/126 (96%)	110 (91%)	10 (8%)	1 (1%)	19 51
44	2m	120/126 (95%)	106 (88%)	13 (11%)	1 (1%)	19 51
45	1n	58/61 (95%)	56 (97%)	2 (3%)	0	100 100
45	2n	58/61 (95%)	52 (90%)	5 (9%)	1 (2%)	9 31
46	1o	86/89 (97%)	79 (92%)	5 (6%)	2 (2%)	6 23
46	2o	86/89 (97%)	76 (88%)	10 (12%)	0	100 100
47	1p	80/88 (91%)	67 (84%)	12 (15%)	1 (1%)	12 37
47	2p	80/88 (91%)	74 (92%)	5 (6%)	1 (1%)	12 37
48	1q	97/105 (92%)	90 (93%)	6 (6%)	1 (1%)	15 45
48	2q	97/105 (92%)	92 (95%)	5 (5%)	0	100 100
49	1r	66/88 (75%)	61 (92%)	4 (6%)	1 (2%)	10 34
49	2r	66/88 (75%)	61 (92%)	5 (8%)	0	100 100
50	1s	81/93 (87%)	69 (85%)	9 (11%)	3 (4%)	3 13
50	2s	81/93 (87%)	66 (82%)	13 (16%)	2 (2%)	5 21
51	1t	94/106 (89%)	84 (89%)	5 (5%)	5 (5%)	2 6
51	2t	94/106 (89%)	83 (88%)	6 (6%)	5 (5%)	2 6
52	1u	21/27 (78%)	19 (90%)	2 (10%)	0	100 100
52	2u	21/27 (78%)	18 (86%)	3 (14%)	0	100 100
All	All	11370/12128 (94%)	10373 (91%)	846 (7%)	151 (1%)	12 37

All (151) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
6	1G	49	ASP
15	1T	118	ARG
26	14	62	ARG
33	1b	10	LEU
33	1b	17	PHE
40	1i	54	ASP
51	1t	10	LEU
5	2F	130	ALA
7	2H	126	PRO
10	2O	5	GLN

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Mol	Chain	Res	Type
26	24	45	GLY
29	27	46	VAL
33	2b	16	HIS
33	2b	123	ALA
35	2d	42	GLN
47	2p	53	VAL
51	2t	10	LEU
4	1E	100	GLU
7	1H	126	PRO
12	1Q	17	LEU
26	14	45	GLY
33	1b	126	GLU
34	1c	107	GLN
35	1d	178	VAL
35	1d	200	GLU
37	1f	40	VAL
47	1p	53	VAL
49	1r	33	ASP
50	1s	29	ARG
51	1t	100	ILE
8	2I	85	GLU
12	2Q	27	VAL
17	2V	79	VAL
26	24	55	ARG
26	24	61	ARG
33	2b	17	PHE
33	2b	125	PRO
34	2c	95	THR
34	2c	156	ARG
35	2d	181	MET
36	2e	77	PRO
40	2i	54	ASP
41	2j	75	ILE
42	2k	49	GLY
50	2s	27	GLU
51	2t	47	GLY
51	2t	95	ALA
20	1Y	54	LYS
20	1Y	103	GLY
21	1Z	159	PRO
26	14	46	GLN
26	14	47	GLN

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Mol	Chain	Res	Type
26	14	53	GLU
33	1b	155	LEU
33	1b	231	GLU
34	1c	81	GLY
41	1j	77	PRO
41	1j	79	ARG
42	1k	49	GLY
50	1s	27	GLU
51	1t	47	GLY
3	2D	3	VAL
4	2E	52	LEU
4	2E	113	PHE
7	2H	47	GLU
8	2I	40	THR
11	2P	38	GLN
13	2R	14	SER
14	2S	84	GLN
20	2Y	43	ASN
21	2Z	163	LEU
23	21	3	LYS
26	24	46	GLN
30	28	7	HIS
38	2g	7	ALA
38	2g	55	GLY
41	2j	78	ASN
44	2m	4	ILE
51	2t	99	LEU
51	2t	100	ILE
4	1E	52	LEU
20	1Y	40	GLU
33	1b	13	ALA
33	1b	20	GLU
35	1d	179	GLU
36	1e	21	ALA
36	1e	85	GLY
41	1j	78	ASN
51	1t	95	ALA
51	1t	102	GLY
6	2G	110	ALA
8	2I	10	GLU
9	2N	2	LYS
15	2T	127	ALA

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Mol	Chain	Res	Type
15	2T	128	GLU
22	20	4	LYS
23	21	45	ASN
26	24	52	THR
33	2b	231	GLU
34	2c	129	ALA
35	2d	18	LYS
36	2e	27	ARG
41	2j	39	PRO
42	2k	105	VAL
45	2n	52	GLN
50	2s	81	ARG
12	1Q	16	ARG
36	1e	69	VAL
38	1g	4	ARG
42	1k	107	SER
48	1q	33	GLY
50	1s	81	ARG
5	2F	21	ALA
11	2P	29	LYS
11	2P	45	LEU
11	2P	140	ALA
15	2T	55	ASN
21	2Z	161	VAL
33	2b	8	LYS
33	2b	20	GLU
33	2b	21	ARG
33	2b	78	GLN
34	2c	3	ASN
38	2g	80	VAL
6	1G	96	ARG
13	1R	107	ASP
19	1X	94	GLY
44	1m	67	GLU
46	1o	19	PRO
7	2H	65	HIS
9	2N	48	MET
21	2Z	146	ILE
34	2c	91	LEU
37	2f	40	VAL
41	2j	77	PRO
34	1c	66	VAL

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Mol	Chain	Res	Type
36	2e	69	VAL
38	1g	80	VAL
42	1k	105	VAL
46	1o	86	GLY
20	2Y	51	VAL
35	2d	5	ILE
36	2e	85	GLY
41	2j	50	ILE
41	1j	91	PRO
3	2D	236	GLY
5	2F	206	ILE
10	2O	72	PRO
14	2S	35	ILE
33	1b	125	PRO

5.3.2 Protein sidechains (i)

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%)	196 (91%)	19 (9%)	10 30
3	2D	215/218 (99%)	190 (88%)	25 (12%)	5 16
4	1E	164/166 (99%)	147 (90%)	17 (10%)	7 21
4	2E	164/166 (99%)	149 (91%)	15 (9%)	9 28
5	1F	160/166 (96%)	142 (89%)	18 (11%)	6 18
5	2F	159/166 (96%)	143 (90%)	16 (10%)	7 23
6	1G	143/156 (92%)	130 (91%)	13 (9%)	9 28
6	2G	143/156 (92%)	122 (85%)	21 (15%)	3 9
7	1H	144/148 (97%)	132 (92%)	12 (8%)	11 32
7	2H	144/148 (97%)	133 (92%)	11 (8%)	13 36
8	1I	113/124 (91%)	97 (86%)	16 (14%)	3 10
8	2I	105/124 (85%)	96 (91%)	9 (9%)	10 30
9	1N	118/119 (99%)	107 (91%)	11 (9%)	9 27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
9	2N	118/119 (99%)	105 (89%)	13 (11%)	6 19
10	1O	100/100 (100%)	95 (95%)	5 (5%)	24 57
10	2O	100/100 (100%)	95 (95%)	5 (5%)	24 57
11	1P	115/116 (99%)	101 (88%)	14 (12%)	5 15
11	2P	115/116 (99%)	108 (94%)	7 (6%)	18 48
12	1Q	111/111 (100%)	104 (94%)	7 (6%)	18 46
12	2Q	111/111 (100%)	98 (88%)	13 (12%)	5 16
13	1R	101/101 (100%)	87 (86%)	14 (14%)	3 10
13	2R	101/101 (100%)	92 (91%)	9 (9%)	9 29
14	1S	86/88 (98%)	78 (91%)	8 (9%)	9 27
14	2S	85/88 (97%)	76 (89%)	9 (11%)	6 20
15	1T	115/127 (91%)	110 (96%)	5 (4%)	29 62
15	2T	113/127 (89%)	106 (94%)	7 (6%)	18 47
16	1U	93/94 (99%)	89 (96%)	4 (4%)	29 62
16	2U	93/94 (99%)	89 (96%)	4 (4%)	29 62
17	1V	80/82 (98%)	69 (86%)	11 (14%)	3 10
17	2V	80/82 (98%)	68 (85%)	12 (15%)	3 9
18	1W	90/92 (98%)	84 (93%)	6 (7%)	16 43
18	2W	90/92 (98%)	82 (91%)	8 (9%)	9 29
19	1X	77/78 (99%)	75 (97%)	2 (3%)	46 77
19	2X	77/78 (99%)	73 (95%)	4 (5%)	23 55
20	1Y	85/91 (93%)	74 (87%)	11 (13%)	4 13
20	2Y	85/91 (93%)	79 (93%)	6 (7%)	14 40
21	1Z	135/179 (75%)	117 (87%)	18 (13%)	4 11
21	2Z	137/179 (76%)	124 (90%)	13 (10%)	8 26
22	10	65/67 (97%)	61 (94%)	4 (6%)	18 47
22	20	65/67 (97%)	61 (94%)	4 (6%)	18 47
23	11	80/83 (96%)	76 (95%)	4 (5%)	24 57
23	21	80/83 (96%)	76 (95%)	4 (5%)	24 57
24	12	65/67 (97%)	61 (94%)	4 (6%)	18 47
24	22	65/67 (97%)	61 (94%)	4 (6%)	18 47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
25	13	51/52 (98%)	46 (90%)	5 (10%)	8 24
25	23	50/52 (96%)	46 (92%)	4 (8%)	12 33
26	14	59/63 (94%)	48 (81%)	11 (19%)	1 5
26	24	53/63 (84%)	46 (87%)	7 (13%)	4 12
27	15	50/52 (96%)	45 (90%)	5 (10%)	7 23
27	25	50/52 (96%)	44 (88%)	6 (12%)	5 15
28	16	51/52 (98%)	47 (92%)	4 (8%)	12 34
28	26	50/52 (96%)	46 (92%)	4 (8%)	12 33
29	17	41/42 (98%)	37 (90%)	4 (10%)	8 24
29	27	41/42 (98%)	38 (93%)	3 (7%)	14 38
30	18	54/55 (98%)	49 (91%)	5 (9%)	9 27
30	28	54/55 (98%)	50 (93%)	4 (7%)	13 38
31	19	34/34 (100%)	33 (97%)	1 (3%)	42 76
31	29	34/34 (100%)	32 (94%)	2 (6%)	19 49
33	1b	192/220 (87%)	170 (88%)	22 (12%)	5 17
33	2b	187/220 (85%)	167 (89%)	20 (11%)	6 20
34	1c	142/188 (76%)	134 (94%)	8 (6%)	21 52
34	2c	140/188 (74%)	129 (92%)	11 (8%)	12 34
35	1d	169/181 (93%)	154 (91%)	15 (9%)	9 29
35	2d	173/181 (96%)	158 (91%)	15 (9%)	10 30
36	1e	113/123 (92%)	108 (96%)	5 (4%)	28 61
36	2e	114/123 (93%)	107 (94%)	7 (6%)	18 48
37	1f	84/90 (93%)	81 (96%)	3 (4%)	35 69
37	2f	85/90 (94%)	81 (95%)	4 (5%)	26 59
38	1g	119/127 (94%)	115 (97%)	4 (3%)	37 71
38	2g	120/127 (94%)	115 (96%)	5 (4%)	30 63
39	1h	114/119 (96%)	105 (92%)	9 (8%)	12 34
39	2h	114/119 (96%)	107 (94%)	7 (6%)	18 48
40	1i	90/99 (91%)	78 (87%)	12 (13%)	4 11
40	2i	89/99 (90%)	78 (88%)	11 (12%)	4 14
41	1j	66/92 (72%)	63 (96%)	3 (4%)	27 61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
41	2j	69/92 (75%)	66 (96%)	3 (4%)	29 62
42	1k	82/99 (83%)	74 (90%)	8 (10%)	8 24
42	2k	83/99 (84%)	79 (95%)	4 (5%)	25 58
43	1l	96/108 (89%)	88 (92%)	8 (8%)	11 32
43	2l	96/108 (89%)	88 (92%)	8 (8%)	11 32
44	1m	93/101 (92%)	84 (90%)	9 (10%)	8 25
44	2m	92/101 (91%)	84 (91%)	8 (9%)	10 30
45	1n	49/50 (98%)	43 (88%)	6 (12%)	5 15
45	2n	49/50 (98%)	43 (88%)	6 (12%)	5 15
46	1o	78/80 (98%)	72 (92%)	6 (8%)	13 35
46	2o	78/80 (98%)	73 (94%)	5 (6%)	17 45
47	1p	69/74 (93%)	65 (94%)	4 (6%)	20 50
47	2p	68/74 (92%)	58 (85%)	10 (15%)	3 9
48	1q	94/97 (97%)	89 (95%)	5 (5%)	22 54
48	2q	94/97 (97%)	89 (95%)	5 (5%)	22 54
49	1r	59/77 (77%)	53 (90%)	6 (10%)	7 22
49	2r	59/77 (77%)	54 (92%)	5 (8%)	10 31
50	1s	69/80 (86%)	65 (94%)	4 (6%)	20 50
50	2s	67/80 (84%)	57 (85%)	10 (15%)	3 9
51	1t	70/82 (85%)	66 (94%)	4 (6%)	20 51
51	2t	70/82 (85%)	68 (97%)	2 (3%)	42 76
52	1u	18/22 (82%)	18 (100%)	0	100 100
52	2u	18/22 (82%)	17 (94%)	1 (6%)	21 52
All	All	9303/10064 (92%)	8508 (92%)	795 (8%)	10 31

All (795) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	32	SER
3	1D	35	LYS
3	1D	61	LEU
3	1D	99	ASP
3	1D	106	ILE
3	1D	113	VAL

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Mol	Chain	Res	Type
3	1D	116	GLN
3	1D	142	VAL
3	1D	154	LYS
3	1D	173	VAL
3	1D	182	LEU
3	1D	211	ARG
3	1D	217	ARG
3	1D	221	VAL
3	1D	229	VAL
3	1D	242	ARG
3	1D	257	LEU
3	1D	260	ARG
3	1D	273	ARG
4	1E	12	THR
4	1E	21	VAL
4	1E	24	THR
4	1E	34	VAL
4	1E	47	VAL
4	1E	73	GLU
4	1E	75	VAL
4	1E	78	LEU
4	1E	82	ARG
4	1E	97	LYS
4	1E	113	PHE
4	1E	116	VAL
4	1E	119	ARG
4	1E	167	VAL
4	1E	170	LEU
4	1E	175	VAL
4	1E	181	LEU
5	1F	12	LEU
5	1F	20	LEU
5	1F	33	LEU
5	1F	43	LYS
5	1F	53	THR
5	1F	57	VAL
5	1F	70	THR
5	1F	74	ARG
5	1F	88	VAL
5	1F	106	ARG
5	1F	125	LEU
5	1F	132	VAL

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Mol	Chain	Res	Type
5	1F	140	LEU
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	7	LEU
6	1G	21	ARG
6	1G	28	VAL
6	1G	43	LEU
6	1G	91	ARG
6	1G	133	LEU
6	1G	135	LEU
6	1G	145	THR
6	1G	148	MET
6	1G	149	VAL
6	1G	159	VAL
6	1G	175	LEU
7	1H	15	VAL
7	1H	33	LEU
7	1H	44	VAL
7	1H	45	VAL
7	1H	50	VAL
7	1H	59	ARG
7	1H	71	LEU
7	1H	101	ARG
7	1H	122	THR
7	1H	134	SER
7	1H	149	ARG
7	1H	155	SER
8	1I	9	LEU
8	1I	12	LEU
8	1I	31	LEU
8	1I	40	THR
8	1I	47	LEU
8	1I	74	ASN
8	1I	77	LEU
8	1I	91	SER
8	1I	92	VAL
8	1I	101	LEU
8	1I	108	THR

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Mol	Chain	Res	Type
8	1I	109	ILE
8	1I	123	LEU
8	1I	140	LEU
8	1I	142	VAL
8	1I	144	VAL
9	1N	28	THR
9	1N	30	ILE
9	1N	33	LEU
9	1N	34	LEU
9	1N	43	THR
9	1N	46	VAL
9	1N	62	VAL
9	1N	67	LEU
9	1N	73	THR
9	1N	87	LEU
9	1N	99	LEU
10	1O	21	CYS
10	1O	31	LYS
10	1O	42	SER
10	1O	89	ASN
10	1O	98	VAL
11	1P	7	ARG
11	1P	15	ARG
11	1P	55	ARG
11	1P	56	SER
11	1P	59	LEU
11	1P	65	ARG
11	1P	83	VAL
11	1P	95	VAL
11	1P	98	GLU
11	1P	101	VAL
11	1P	112	LEU
11	1P	125	VAL
11	1P	126	VAL
11	1P	133	SER
12	1Q	7	MET
12	1Q	35	VAL
12	1Q	56	ARG
12	1Q	75	THR
12	1Q	109	VAL
12	1Q	110	THR
12	1Q	133	ARG

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Mol	Chain	Res	Type
13	1R	6	SER
13	1R	8	ARG
13	1R	15	SER
13	1R	29	LEU
13	1R	33	ARG
13	1R	36	THR
13	1R	44	LEU
13	1R	54	LEU
13	1R	67	LEU
13	1R	79	LEU
13	1R	100	LEU
13	1R	102	GLU
13	1R	111	LEU
13	1R	114	VAL
14	1S	8	GLU
14	1S	17	ARG
14	1S	19	LYS
14	1S	25	ARG
14	1S	36	TYR
14	1S	71	ARG
14	1S	85	VAL
14	1S	110	LEU
15	1T	6	LEU
15	1T	28	VAL
15	1T	49	VAL
15	1T	51	ARG
15	1T	118	ARG
16	1U	8	VAL
16	1U	31	SER
16	1U	74	LEU
16	1U	95	LEU
17	1V	7	THR
17	1V	18	LEU
17	1V	46	VAL
17	1V	51	VAL
17	1V	52	VAL
17	1V	62	LEU
17	1V	72	VAL
17	1V	73	SER
17	1V	79	VAL
17	1V	82	ARG
17	1V	95	LEU

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Mol	Chain	Res	Type
18	1W	11	ARG
18	1W	23	LEU
18	1W	60	ASN
18	1W	90	ARG
18	1W	92	ARG
18	1W	107	LEU
19	1X	35	THR
19	1X	57	LEU
20	1Y	11	ASP
20	1Y	28	LYS
20	1Y	43	ASN
20	1Y	49	VAL
20	1Y	50	ARG
20	1Y	55	TYR
20	1Y	61	ILE
20	1Y	72	VAL
20	1Y	90	LEU
20	1Y	106	LEU
20	1Y	107	ASP
21	1Z	1	MET
21	1Z	18	LEU
21	1Z	33	LEU
21	1Z	42	VAL
21	1Z	56	VAL
21	1Z	61	LEU
21	1Z	70	LEU
21	1Z	76	LEU
21	1Z	84	GLU
21	1Z	91	LEU
21	1Z	102	LEU
21	1Z	124	ILE
21	1Z	126	VAL
21	1Z	149	SER
21	1Z	154	ASP
21	1Z	155	LEU
21	1Z	161	VAL
21	1Z	171	ILE
22	10	10	THR
22	10	14	ARG
22	10	37	LEU
22	10	74	ARG
23	11	30	VAL

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Mol	Chain	Res	Type
23	11	35	THR
23	11	56	GLN
23	11	95	LEU
24	12	19	VAL
24	12	45	SER
24	12	53	LEU
24	12	69	ARG
25	13	3	ARG
25	13	34	GLU
25	13	54	VAL
25	13	58	VAL
25	13	60	GLU
26	14	3	GLU
26	14	23	GLU
26	14	46	GLN
26	14	49	PHE
26	14	50	VAL
26	14	52	THR
26	14	53	GLU
26	14	56	VAL
26	14	63	TYR
26	14	66	SER
26	14	67	TYR
27	15	6	VAL
27	15	16	ARG
27	15	29	THR
27	15	55	ARG
27	15	58	LEU
28	16	6	ARG
28	16	19	ARG
28	16	24	GLU
28	16	48	VAL
29	17	1	MET
29	17	4	THR
29	17	24	THR
29	17	43	THR
30	18	14	VAL
30	18	23	VAL
30	18	31	HIS
30	18	32	LEU
30	18	34	TRP
31	19	7	VAL

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Mol	Chain	Res	Type
33	1b	21	ARG
33	1b	23	ARG
33	1b	24	TRP
33	1b	67	THR
33	1b	94	ASN
33	1b	107	THR
33	1b	111	ARG
33	1b	112	VAL
33	1b	122	PHE
33	1b	126	GLU
33	1b	127	ILE
33	1b	158	LEU
33	1b	164	VAL
33	1b	170	GLU
33	1b	179	LYS
33	1b	185	ILE
33	1b	187	LEU
33	1b	192	SER
33	1b	196	LEU
33	1b	208	ILE
33	1b	223	ILE
33	1b	233	SER
34	1c	3	ASN
34	1c	15	THR
34	1c	21	ARG
34	1c	110	ASN
34	1c	112	SER
34	1c	115	LEU
34	1c	172	ARG
34	1c	195	VAL
35	1d	5	ILE
35	1d	19	LEU
35	1d	22	LYS
35	1d	31	CYS
35	1d	49	ARG
35	1d	76	ARG
35	1d	83	SER
35	1d	135	LEU
35	1d	144	ASP
35	1d	158	ILE
35	1d	175	SER
35	1d	177	ASP

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Mol	Chain	Res	Type
35	1d	178	VAL
35	1d	194	LEU
35	1d	205	GLU
36	1e	24	ARG
36	1e	31	LEU
36	1e	41	VAL
36	1e	81	GLU
36	1e	91	LEU
37	1f	64	GLN
37	1f	75	LEU
37	1f	81	ILE
38	1g	12	LEU
38	1g	51	GLN
38	1g	113	GLU
38	1g	114	ARG
39	1h	19	VAL
39	1h	26	VAL
39	1h	29	SER
39	1h	38	ILE
39	1h	52	ASP
39	1h	82	HIS
39	1h	85	ARG
39	1h	104	ARG
39	1h	133	LEU
40	1i	9	ARG
40	1i	23	ASN
40	1i	42	ARG
40	1i	54	ASP
40	1i	64	THR
40	1i	65	VAL
40	1i	74	ILE
40	1i	83	ARG
40	1i	92	TYR
40	1i	108	VAL
40	1i	121	ARG
40	1i	128	ARG
41	1j	8	LEU
41	1j	38	ILE
41	1j	58	ASP
42	1k	14	VAL
42	1k	16	SER
42	1k	31	THR

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Mol	Chain	Res	Type
42	1k	33	THR
42	1k	48	ILE
42	1k	109	VAL
42	1k	114	VAL
42	1k	126	ARG
43	1l	27	LEU
43	1l	33	ARG
43	1l	58	VAL
43	1l	83	VAL
43	1l	85	ILE
43	1l	89	ARG
43	1l	113	ARG
43	1l	117	ARG
44	1m	4	ILE
44	1m	14	ARG
44	1m	19	LEU
44	1m	64	TRP
44	1m	102	ARG
44	1m	103	THR
44	1m	109	THR
44	1m	117	VAL
44	1m	122	LYS
45	1n	3	ARG
45	1n	13	THR
45	1n	18	VAL
45	1n	26	ARG
45	1n	29	ARG
45	1n	33	VAL
46	1o	7	GLU
46	1o	21	ASP
46	1o	39	LEU
46	1o	64	ARG
46	1o	66	LEU
46	1o	87	ILE
47	1p	19	ILE
47	1p	61	SER
47	1p	67	THR
47	1p	69	THR
48	1q	6	LEU
48	1q	35	VAL
48	1q	39	SER
48	1q	45	HIS

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Mol	Chain	Res	Type
48	1q	93	GLN
49	1r	31	LEU
49	1r	37	VAL
49	1r	46	GLU
49	1r	59	SER
49	1r	76	LEU
49	1r	85	LEU
50	1s	12	ASP
50	1s	41	VAL
50	1s	48	THR
50	1s	79	THR
51	1t	10	LEU
51	1t	13	LEU
51	1t	31	SER
51	1t	84	LEU
3	2D	10	THR
3	2D	12	SER
3	2D	14	ARG
3	2D	38	LYS
3	2D	69	ARG
3	2D	88	ARG
3	2D	94	LEU
3	2D	103	ARG
3	2D	106	ILE
3	2D	113	VAL
3	2D	115	GLN
3	2D	134	ARG
3	2D	136	ILE
3	2D	142	VAL
3	2D	157	ARG
3	2D	169	GLU
3	2D	176	ARG
3	2D	183	ARG
3	2D	211	ARG
3	2D	221	VAL
3	2D	229	VAL
3	2D	242	ARG
3	2D	259	THR
3	2D	260	ARG
3	2D	276	LYS
4	2E	7	VAL
4	2E	9	VAL

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Mol	Chain	Res	Type
4	2E	21	VAL
4	2E	34	VAL
4	2E	38	THR
4	2E	45	THR
4	2E	75	VAL
4	2E	78	LEU
4	2E	105	THR
4	2E	113	PHE
4	2E	116	VAL
4	2E	119	ARG
4	2E	121	ASN
4	2E	175	VAL
4	2E	181	LEU
5	2F	20	LEU
5	2F	32	LEU
5	2F	33	LEU
5	2F	50	SER
5	2F	74	ARG
5	2F	88	VAL
5	2F	95	ARG
5	2F	106	ARG
5	2F	110	LEU
5	2F	132	VAL
5	2F	158	THR
5	2F	165	ARG
5	2F	183	VAL
5	2F	192	LEU
5	2F	197	ASP
5	2F	201	VAL
6	2G	3	LEU
6	2G	5	VAL
6	2G	14	GLU
6	2G	18	GLU
6	2G	27	ASN
6	2G	31	VAL
6	2G	43	LEU
6	2G	45	GLU
6	2G	49	ASP
6	2G	60	LEU
6	2G	79	ASN
6	2G	91	ARG
6	2G	113	ARG

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Mol	Chain	Res	Type
6	2G	115	ARG
6	2G	126	ASP
6	2G	135	LEU
6	2G	140	ILE
6	2G	145	THR
6	2G	152	LEU
6	2G	159	VAL
6	2G	175	LEU
7	2H	3	ARG
7	2H	45	VAL
7	2H	56	SER
7	2H	57	ASP
7	2H	63	SER
7	2H	71	LEU
7	2H	84	SER
7	2H	88	LEU
7	2H	121	ILE
7	2H	148	ILE
7	2H	175	LYS
8	2I	38	LEU
8	2I	77	LEU
8	2I	92	VAL
8	2I	116	LEU
8	2I	121	LYS
8	2I	129	THR
8	2I	140	LEU
8	2I	144	VAL
8	2I	145	VAL
9	2N	5	VAL
9	2N	14	VAL
9	2N	34	LEU
9	2N	38	HIS
9	2N	43	THR
9	2N	46	VAL
9	2N	58	ASP
9	2N	62	VAL
9	2N	85	ILE
9	2N	87	LEU
9	2N	99	LEU
9	2N	112	LEU
9	2N	140	VAL
10	2O	17	ARG

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Mol	Chain	Res	Type
10	2O	24	VAL
10	2O	35	VAL
10	2O	69	ILE
10	2O	70	LYS
11	2P	42	SER
11	2P	45	LEU
11	2P	56	SER
11	2P	83	VAL
11	2P	95	VAL
11	2P	99	LEU
11	2P	112	LEU
12	2Q	1	MET
12	2Q	11	LYS
12	2Q	16	ARG
12	2Q	21	THR
12	2Q	38	GLU
12	2Q	55	VAL
12	2Q	75	THR
12	2Q	85	LYS
12	2Q	98	LYS
12	2Q	109	VAL
12	2Q	110	THR
12	2Q	133	ARG
12	2Q	139	GLU
13	2R	6	SER
13	2R	18	LEU
13	2R	24	GLN
13	2R	27	SER
13	2R	29	LEU
13	2R	33	ARG
13	2R	65	LEU
13	2R	100	LEU
13	2R	111	LEU
14	2S	21	THR
14	2S	25	ARG
14	2S	26	LEU
14	2S	27	SER
14	2S	36	TYR
14	2S	53	SER
14	2S	75	GLU
14	2S	78	LEU
14	2S	110	LEU

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Mol	Chain	Res	Type
15	2T	31	SER
15	2T	63	VAL
15	2T	74	ARG
15	2T	89	VAL
15	2T	90	GLN
15	2T	96	ARG
15	2T	108	ARG
16	2U	30	LYS
16	2U	31	SER
16	2U	55	ARG
16	2U	74	LEU
17	2V	7	THR
17	2V	32	THR
17	2V	43	GLU
17	2V	46	VAL
17	2V	51	VAL
17	2V	61	VAL
17	2V	62	LEU
17	2V	73	SER
17	2V	79	VAL
17	2V	82	ARG
17	2V	85	LYS
17	2V	99	ILE
18	2W	1	MET
18	2W	11	ARG
18	2W	15	ARG
18	2W	17	VAL
18	2W	23	LEU
18	2W	67	ASP
18	2W	96	ILE
18	2W	109	GLU
19	2X	1	MET
19	2X	48	LYS
19	2X	56	THR
19	2X	57	LEU
20	2Y	6	HIS
20	2Y	40	GLU
20	2Y	49	VAL
20	2Y	97	ARG
20	2Y	99	CYS
20	2Y	107	ASP
21	2Z	5	LEU

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Mol	Chain	Res	Type
21	2Z	24	LEU
21	2Z	33	LEU
21	2Z	42	VAL
21	2Z	52	SER
21	2Z	70	LEU
21	2Z	98	MET
21	2Z	123	ASP
21	2Z	129	SER
21	2Z	150	LEU
21	2Z	153	SER
21	2Z	154	ASP
21	2Z	171	ILE
22	20	9	SER
22	20	10	THR
22	20	14	ARG
22	20	68	GLU
23	21	4	VAL
23	21	61	ARG
23	21	89	GLU
23	21	95	LEU
24	22	26	ARG
24	22	53	LEU
24	22	66	GLU
24	22	70	GLN
25	23	18	ASP
25	23	23	LEU
25	23	30	ARG
25	23	54	VAL
26	24	10	VAL
26	24	24	THR
26	24	34	GLU
26	24	49	PHE
26	24	50	VAL
26	24	59	PHE
26	24	63	TYR
27	25	6	VAL
27	25	16	ARG
27	25	29	THR
27	25	33	CYS
27	25	48	GLU
27	25	58	LEU
28	26	9	LEU

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Mol	Chain	Res	Type
28	26	23	THR
28	26	29	ASN
28	26	51	GLU
29	27	23	ARG
29	27	39	ARG
29	27	41	ARG
30	28	13	ARG
30	28	31	HIS
30	28	32	LEU
30	28	34	TRP
31	29	7	VAL
31	29	26	ILE
33	2b	7	VAL
33	2b	11	LEU
33	2b	47	THR
33	2b	48	MET
33	2b	49	GLU
33	2b	56	ARG
33	2b	67	THR
33	2b	87	ARG
33	2b	94	ASN
33	2b	102	LEU
33	2b	115	LEU
33	2b	126	GLU
33	2b	127	ILE
33	2b	135	GLN
33	2b	140	HIS
33	2b	178	ARG
33	2b	189	ASP
33	2b	195	ASP
33	2b	221	LEU
33	2b	235	SER
34	2c	15	THR
34	2c	32	LEU
34	2c	47	LEU
34	2c	57	ILE
34	2c	70	VAL
34	2c	152	ILE
34	2c	166	GLU
34	2c	178	LEU
34	2c	179	ARG
34	2c	188	LEU

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Mol	Chain	Res	Type
34	2c	190	ARG
35	2d	12	CYS
35	2d	31	CYS
35	2d	59	ARG
35	2d	83	SER
35	2d	107	ARG
35	2d	127	THR
35	2d	135	LEU
35	2d	150	GLU
35	2d	155	LEU
35	2d	158	ILE
35	2d	170	VAL
35	2d	175	SER
35	2d	194	LEU
35	2d	205	GLU
35	2d	208	SER
36	2e	13	ILE
36	2e	31	LEU
36	2e	41	VAL
36	2e	72	GLN
36	2e	90	VAL
36	2e	91	LEU
36	2e	111	GLU
37	2f	1	MET
37	2f	21	LEU
37	2f	59	TYR
37	2f	72	VAL
38	2g	15	ASP
38	2g	16	LEU
38	2g	52	GLU
38	2g	79	ARG
38	2g	98	SER
39	2h	2	LEU
39	2h	39	LEU
39	2h	51	VAL
39	2h	63	LEU
39	2h	104	ARG
39	2h	119	LEU
39	2h	127	LEU
40	2i	27	THR
40	2i	50	LEU
40	2i	53	VAL

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Mol	Chain	Res	Type
40	2i	64	THR
40	2i	65	VAL
40	2i	89	ASN
40	2i	93	ARG
40	2i	102	LEU
40	2i	108	VAL
40	2i	125	TYR
40	2i	128	ARG
41	2j	8	LEU
41	2j	16	LEU
41	2j	100	THR
42	2k	14	VAL
42	2k	41	THR
42	2k	96	ARG
42	2k	114	VAL
43	2l	22	SER
43	2l	33	ARG
43	2l	36	VAL
43	2l	83	VAL
43	2l	86	ARG
43	2l	97	ARG
43	2l	113	ARG
43	2l	123	LYS
44	2m	3	ARG
44	2m	15	VAL
44	2m	19	LEU
44	2m	27	LYS
44	2m	47	ASP
44	2m	50	GLU
44	2m	64	TRP
44	2m	86	CYS
45	2n	3	ARG
45	2n	6	LEU
45	2n	22	THR
45	2n	32	SER
45	2n	33	VAL
45	2n	56	VAL
46	2o	38	ARG
46	2o	39	LEU
46	2o	58	MET
46	2o	65	ARG
46	2o	87	ILE

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Mol	Chain	Res	Type
47	2p	2	VAL
47	2p	20	VAL
47	2p	21	VAL
47	2p	42	ARG
47	2p	45	THR
47	2p	53	VAL
47	2p	60	LEU
47	2p	62	VAL
47	2p	67	THR
47	2p	69	THR
48	2q	6	LEU
48	2q	7	THR
48	2q	24	GLU
48	2q	35	VAL
48	2q	83	ASP
49	2r	25	THR
49	2r	26	LEU
49	2r	37	VAL
49	2r	46	GLU
49	2r	65	ILE
50	2s	5	LEU
50	2s	12	ASP
50	2s	33	THR
50	2s	36	ARG
50	2s	41	VAL
50	2s	48	THR
50	2s	49	ILE
50	2s	65	ASN
50	2s	77	THR
50	2s	83	HIS
51	2t	62	LEU
51	2t	71	THR
52	2u	7	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (93) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	126	GLN
4	1E	48	GLN
5	1F	8	GLN
5	1F	69	HIS
7	1H	147	ASN

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Mol	Chain	Res	Type
10	1O	89	ASN
12	1Q	12	GLN
13	1R	13	HIS
13	1R	91	GLN
16	1U	81	HIS
16	1U	94	ASN
19	1X	31	HIS
19	1X	82	GLN
20	1Y	6	HIS
21	1Z	32	HIS
21	1Z	73	GLN
21	1Z	151	HIS
23	11	56	GLN
24	12	9	GLN
27	15	23	HIS
33	1b	40	HIS
33	1b	94	ASN
34	1c	6	HIS
34	1c	37	GLN
34	1c	162	GLN
34	1c	176	HIS
35	1d	42	GLN
35	1d	77	ASN
35	1d	116	GLN
35	1d	119	GLN
35	1d	123	HIS
35	1d	125	HIS
36	1e	78	HIS
37	1f	73	ASN
37	1f	100	ASN
38	1g	13	GLN
38	1g	28	ASN
38	1g	51	GLN
38	1g	122	HIS
40	1i	3	GLN
40	1i	23	ASN
40	1i	89	ASN
40	1i	124	GLN
41	1j	56	HIS
43	1l	99	HIS
46	1o	46	HIS
47	1p	13	HIS

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Mol	Chain	Res	Type
48	1q	26	GLN
50	1s	83	HIS
3	2D	116	GLN
4	2E	48	GLN
6	2G	132	ASN
9	2N	131	GLN
10	2O	5	GLN
12	2Q	12	GLN
12	2Q	13	GLN
12	2Q	123	HIS
14	2S	38	GLN
16	2U	94	ASN
17	2V	64	HIS
18	2W	61	ASN
19	2X	31	HIS
19	2X	82	GLN
21	2Z	34	ASN
21	2Z	73	GLN
23	21	56	GLN
24	22	70	GLN
30	28	35	GLN
31	29	36	GLN
33	2b	40	HIS
33	2b	78	GLN
33	2b	94	ASN
33	2b	95	GLN
34	2c	37	GLN
34	2c	176	HIS
35	2d	77	ASN
35	2d	116	GLN
35	2d	125	HIS
35	2d	161	ASN
36	2e	20	GLN
38	2g	28	ASN
40	2i	3	GLN
40	2i	31	GLN
40	2i	58	HIS
40	2i	89	ASN
41	2j	13	HIS
44	2m	40	ASN
44	2m	62	ASN
46	2o	28	GLN

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Mol	Chain	Res	Type
46	2o	62	GLN
50	2s	23	ASN
50	2s	47	HIS
50	2s	69	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2861/2915 (98%)	458 (16%)	29 (1%)
1	2A	2788/2915 (95%)	493 (17%)	23 (0%)
2	1B	120/121 (99%)	9 (7%)	1 (0%)
2	2B	118/121 (97%)	33 (27%)	0
32	1a	1494/1521 (98%)	235 (15%)	0
32	2a	1498/1521 (98%)	288 (19%)	0
53	1v	12/24 (50%)	1 (8%)	0
53	2v	12/24 (50%)	4 (33%)	0
54	1w	71/76 (93%)	21 (29%)	0
54	1y	71/76 (93%)	24 (33%)	0
54	2w	68/76 (89%)	24 (35%)	0
54	2y	69/76 (90%)	23 (33%)	0
55	1x	75/77 (97%)	9 (12%)	0
55	2x	75/77 (97%)	14 (18%)	0
All	All	9332/9620 (97%)	1636 (17%)	53 (0%)

All (1636) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	13	A
1	1A	15	G
1	1A	34	C
1	1A	45	C
1	1A	50	G
1	1A	70	A
1	1A	71	U
1	1A	73	A
1	1A	74	G
1	1A	83	A
1	1A	90	A
1	1A	116	A
1	1A	117	A

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Mol	Chain	Res	Type
1	1A	118	U
1	1A	123	G
1	1A	139	A
1	1A	155	C
1	1A	171	A
1	1A	185	A
1	1A	188	A
1	1A	194	G
1	1A	203	G
1	1A	205	A
1	1A	211	A
1	1A	212	A
1	1A	214	A
1	1A	217	A
1	1A	218	A
1	1A	237	G
1	1A	258	U
1	1A	271	U
1	1A	272	U
1	1A	273	G
1	1A	289	G
1	1A	296	U
1	1A	303	C
1	1A	335	A
1	1A	353	G
1	1A	354	A
1	1A	369	A
1	1A	376	G
1	1A	387	G
1	1A	388	A
1	1A	389	G
1	1A	407	U
1	1A	413	G
1	1A	423	G
1	1A	432	U
1	1A	438	G
1	1A	439	A
1	1A	455	A
1	1A	470	C
1	1A	474	U
1	1A	483	A
1	1A	507	G

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Mol	Chain	Res	Type
1	1A	526	A
1	1A	529	U
1	1A	530	A
1	1A	534	C
1	1A	555	G
1	1A	556	C
1	1A	557	A
1	1A	558	G
1	1A	569	G
1	1A	573	G
1	1A	586	G
1	1A	596	G
1	1A	598	A
1	1A	609	A
1	1A	616	G
1	1A	626	A
1	1A	627	G
1	1A	630	U
1	1A	639	G
1	1A	641	G
1	1A	644	G
1	1A	652	A
1	1A	662	A
1	1A	671	A
1	1A	693	G
1	1A	697	C
1	1A	716	G
1	1A	733	G
1	1A	761	U
1	1A	764	G
1	1A	777	C
1	1A	811	A
1	1A	822	G
1	1A	823	G
1	1A	829	A
1	1A	830	A
1	1A	831	A
1	1A	832	G
1	1A	839	G
1	1A	852	G
1	1A	859	C
1	1A	866	A

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Mol	Chain	Res	Type
1	1A	874	U
1	1A	875	U
1	1A	879	G
1	1A	902	G
1	1A	906	G
1	1A	913	A
1	1A	926	G
1	1A	927	G
1	1A	931	C
1	1A	932	C
1	1A	933	C
1	1A	934	A
1	1A	935	C
1	1A	936	C
1	1A	937	A
1	1A	938	G
1	1A	942	A
1	1A	943	C
1	1A	944	C
1	1A	946	A
1	1A	953	U
1	1A	956	A
1	1A	961	C
1	1A	976	G
1	1A	977	G
1	1A	983	G
1	1A	990	A
1	1A	991	G
1	1A	998	A
1	1A	1003	U
1	1A	1006	C
1	1A	1019	G
1	1A	1020	C
1	1A	1021	G
1	1A	1029	A
1	1A	1031	C
1	1A	1042	A
1	1A	1058	U
1	1A	1059	C
1	1A	1071	G
1	1A	1072	U
1	1A	1073	A

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Mol	Chain	Res	Type
1	1A	1079	U
1	1A	1083	G
1	1A	1084	C
1	1A	1090	G
1	1A	1091	A
1	1A	1092	A
1	1A	1093	G
1	1A	1094	A
1	1A	1100	A
1	1A	1101	G
1	1A	1104	G
1	1A	1109	G
1	1A	1114	G
1	1A	1116	A
1	1A	1117	G
1	1A	1119	A
1	1A	1120	G
1	1A	1121	C
1	1A	1122	C
1	1A	1124	U
1	1A	1125	C
1	1A	1127	U
1	1A	1132	A
1	1A	1134	A
1	1A	1135	G
1	1A	1136	U
1	1A	1140	U
1	1A	1142	A
1	1A	1147	U
1	1A	1149	A
1	1A	1154	U
1	1A	1156	G
1	1A	1157	A
1	1A	1158	G
1	1A	1162	C
1	1A	1175	A
1	1A	1176	U
1	1A	1180	C
1	1A	1181	G
1	1A	1187	U
1	1A	1201	A
1	1A	1216	G

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Mol	Chain	Res	Type
1	1A	1217	G
1	1A	1218	G
1	1A	1219	A
1	1A	1220	U
1	1A	1221	G
1	1A	1222	A
1	1A	1223	C
1	1A	1263	C
1	1A	1275	G
1	1A	1282	G
1	1A	1283	A
1	1A	1296	G
1	1A	1299	A
1	1A	1302	G
1	1A	1314	A
1	1A	1317	G
1	1A	1318	A
1	1A	1319	U
1	1A	1327	G
1	1A	1346	U
1	1A	1347	A
1	1A	1366	C
1	1A	1398	U
1	1A	1405	A
1	1A	1406	A
1	1A	1411	A
1	1A	1430	A
1	1A	1431	G
1	1A	1441	A
1	1A	1442	U
1	1A	1462	G
1	1A	1463	C
1	1A	1466	U
1	1A	1467	G
1	1A	1474	C
1	1A	1475	G
1	1A	1491	A
1	1A	1497	G
1	1A	1502	G
1	1A	1514	C
1	1A	1529	G
1	1A	1539	C

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Mol	Chain	Res	Type
1	1A	1554	A
1	1A	1555	C
1	1A	1556	A
1	1A	1562	U
1	1A	1605	A
1	1A	1606	G
1	1A	1613	A
1	1A	1616	A
1	1A	1625	U
1	1A	1627	A
1	1A	1628	G
1	1A	1631	C
1	1A	1632	A
1	1A	1654	A
1	1A	1655	A
1	1A	1656	A
1	1A	1695	C
1	1A	1721	G
1	1A	1743	G
1	1A	1747	A
1	1A	1748	A
1	1A	1750	G
1	1A	1764	G
1	1A	1767	A
1	1A	1787	G
1	1A	1794	G
1	1A	1795	G
1	1A	1804	A
1	1A	1807	G
1	1A	1811	A
1	1A	1813	C
1	1A	1822	A
1	1A	1828	C
1	1A	1831	C
1	1A	1832	G
1	1A	1833	A
1	1A	1843	A
1	1A	1847	G
1	1A	1860	A
1	1A	1870	G
1	1A	1878	A
1	1A	1892	G

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Mol	Chain	Res	Type
1	1A	1899	A
1	1A	1900	G
1	1A	1911	A
1	1A	1922	A
1	1A	1928	G
1	1A	1935	A
1	1A	1940	A
1	1A	1941	A
1	1A	1951	G
1	1A	1952	G
1	1A	1956	C
1	1A	1959	A
1	1A	1960	A
1	1A	1977	U
1	1A	1985	U
1	1A	1988	A
1	1A	1989	C
1	1A	1992	A
1	1A	1993	A
1	1A	1994	A
1	1A	2005	C
1	1A	2014	G
1	1A	2015	U
1	1A	2019	G
1	1A	2042	A
1	1A	2045	G
1	1A	2053	A
1	1A	2055	A
1	1A	2061	C
1	1A	2065	C
1	1A	2071	G
1	1A	2074	G
1	1A	2077	C
1	1A	2078	G
1	1A	2082	A
1	1A	2083	G
1	1A	2084	A
1	1A	2091	G
1	1A	2115	G
1	1A	2120	U
1	1A	2128	G
1	1A	2132	G

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Mol	Chain	Res	Type
1	1A	2135	U
1	1A	2136	A
1	1A	2138	G
1	1A	2143	G
1	1A	2148	A
1	1A	2149	G
1	1A	2151	C
1	1A	2152	U
1	1A	2153	G
1	1A	2154	U
1	1A	2155	G
1	1A	2156	A
1	1A	2157	A
1	1A	2158	C
1	1A	2162	C
1	1A	2164	C
1	1A	2166	U
1	1A	2168	C
1	1A	2169	G
1	1A	2170	G
1	1A	2172	U
1	1A	2173	G
1	1A	2178	G
1	1A	2179	G
1	1A	2180	A
1	1A	2181	G
1	1A	2184	G
1	1A	2188	G
1	1A	2189	U
1	1A	2193	A
1	1A	2194	U
1	1A	2195	A
1	1A	2196	C
1	1A	2200	C
1	1A	2204	G
1	1A	2206	G
1	1A	2214	G
1	1A	2220	A
1	1A	2227	G
1	1A	2228	G
1	1A	2229	A
1	1A	2230	U

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Mol	Chain	Res	Type
1	1A	2237	A
1	1A	2247	G
1	1A	2250	G
1	1A	2251	G
1	1A	2280	A
1	1A	2291	G
1	1A	2292	G
1	1A	2295	C
1	1A	2298	A
1	1A	2299	A
1	1A	2306	C
1	1A	2308	U
1	1A	2317	A
1	1A	2319	G
1	1A	2320	G
1	1A	2324	U
1	1A	2326	C
1	1A	2332	A
1	1A	2333	G
1	1A	2334	A
1	1A	2337	G
1	1A	2346	G
1	1A	2348	A
1	1A	2359	C
1	1A	2362	C
1	1A	2365	G
1	1A	2366	G
1	1A	2373	A
1	1A	2389	A
1	1A	2391	G
1	1A	2395	G
1	1A	2397	C
1	1A	2414	C
1	1A	2418	U
1	1A	2422	G
1	1A	2436	C
1	1A	2437	A
1	1A	2440	G
1	1A	2441	G
1	1A	2442	A
1	1A	2443	U
1	1A	2446	A

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Mol	Chain	Res	Type
1	1A	2447	A
1	1A	2451	A
1	1A	2452	C
1	1A	2453	C
1	1A	2460	A
1	1A	2483	C
1	1A	2488	A
1	1A	2493	G
1	1A	2502	G
1	1A	2514	G
1	1A	2517	G
1	1A	2518	U
1	1A	2530	A
1	1A	2532	C
1	1A	2541	G
1	1A	2566	U
1	1A	2578	A
1	1A	2579	G
1	1A	2585	C
1	1A	2586	G
1	1A	2594	G
1	1A	2597	U
1	1A	2614	A
1	1A	2621	U
1	1A	2623	U
1	1A	2624	C
1	1A	2640	C
1	1A	2641	A
1	1A	2642	G
1	1A	2666	A
1	1A	2701	U
1	1A	2702	C
1	1A	2714	U
1	1A	2715	C
1	1A	2725	A
1	1A	2726	A
1	1A	2727	G
1	1A	2739	U
1	1A	2746	A
1	1A	2753	A
1	1A	2777	A
1	1A	2778	A

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Mol	Chain	Res	Type
1	1A	2779	G
1	1A	2782	C
1	1A	2791	A
1	1A	2793	G
1	1A	2802	C
1	1A	2803	A
1	1A	2804	C
1	1A	2806	G
1	1A	2807	C
1	1A	2813	G
1	1A	2814	C
1	1A	2828	G
1	1A	2830	A
1	1A	2831	A
1	1A	2843	G
1	1A	2845	A
1	1A	2847	G
1	1A	2871	G
1	1A	2882	G
1	1A	2883	A
1	1A	2890	C
1	1A	2899	C
1	1A	2901	A
1	1A	2903	G
2	1B	2	C
2	1B	24	G
2	1B	35	U
2	1B	42	C
2	1B	56	G
2	1B	67	G
2	1B	73	A
2	1B	106	G
2	1B	110	G
32	1a	7	G
32	1a	9	G
32	1a	32	A
32	1a	39	G
32	1a	47	C
32	1a	48	C
32	1a	51	A
32	1a	54	C
32	1a	61	G

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Mol	Chain	Res	Type
32	1a	73	G
32	1a	79	G
32	1a	91	C
32	1a	98	G
32	1a	116	A
32	1a	121	C
32	1a	131	C
32	1a	144	G
32	1a	163	C
32	1a	171	A
32	1a	174	C
32	1a	182	U
32	1a	189(F)	U
32	1a	189(G)	G
32	1a	189(J)	G
32	1a	195	A
32	1a	197	A
32	1a	199	G
32	1a	201	C
32	1a	202	U
32	1a	203	U
32	1a	204	U
32	1a	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	301	G
32	1a	306	G
32	1a	328	C
32	1a	332	G
32	1a	342	C
32	1a	344	A
32	1a	345	C
32	1a	347	G
32	1a	348	G
32	1a	352	C
32	1a	353	A

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Mol	Chain	Res	Type
32	1a	354	G
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	384	G
32	1a	397	A
32	1a	398	C
32	1a	406	G
32	1a	412	A
32	1a	413	G
32	1a	423	G
32	1a	424	G
32	1a	429	U
32	1a	430	A
32	1a	439	A
32	1a	441	A
32	1a	442	C
32	1a	452	A
32	1a	461	A
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	519	C
32	1a	527	7MG
32	1a	531	U
32	1a	532	A
32	1a	536	C
32	1a	544	G
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

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Mol	Chain	Res	Type
32	1a	592	G
32	1a	596	C
32	1a	630	G
32	1a	653	A
32	1a	659	U
32	1a	665	A
32	1a	673	G
32	1a	687	A
32	1a	688	G
32	1a	695	A
32	1a	721	G
32	1a	723	U
32	1a	731	G
32	1a	747	C
32	1a	749	C
32	1a	753	A
32	1a	755	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	874	G
32	1a	885	G
32	1a	902	G
32	1a	914	A
32	1a	926	G
32	1a	927	G
32	1a	934	C
32	1a	935	A
32	1a	960	U
32	1a	961	U
32	1a	968	A

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Mol	Chain	Res	Type
32	1a	969	A
32	1a	971	G
32	1a	974	A
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	992	U
32	1a	993	G
32	1a	1000	U
32	1a	1003	G
32	1a	1005	A
32	1a	1006	C
32	1a	1009	G
32	1a	1020	U
32	1a	1022	G
32	1a	1023	G
32	1a	1025	U
32	1a	1026	G
32	1a	1027	C
32	1a	1030	C
32	1a	1030(A)	G
32	1a	1030(C)	G
32	1a	1031	G
32	1a	1033	G
32	1a	1039	C
32	1a	1043	C
32	1a	1045	C
32	1a	1046	A
32	1a	1053	G
32	1a	1054	C
32	1a	1065	U
32	1a	1066	C
32	1a	1068	G
32	1a	1081	G
32	1a	1094	G
32	1a	1095	U
32	1a	1096	C
32	1a	1101	A
32	1a	1108	G
32	1a	1125	U
32	1a	1132	C
32	1a	1134	G

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Mol	Chain	Res	Type
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	1159	U
32	1a	1184	G
32	1a	1196	U
32	1a	1197	G
32	1a	1201	A
32	1a	1202	G
32	1a	1212	U
32	1a	1213	A
32	1a	1214	C
32	1a	1227	A
32	1a	1236	A
32	1a	1238	A
32	1a	1256	A
32	1a	1257	U
32	1a	1270	C
32	1a	1273	G
32	1a	1278	U
32	1a	1279	A
32	1a	1280	A
32	1a	1286	A
32	1a	1287	A
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1322	C
32	1a	1338	G
32	1a	1346	A
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1370	G
32	1a	1378	C
32	1a	1397	C
32	1a	1406	U
32	1a	1419	G

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Mol	Chain	Res	Type
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1446	U
32	1a	1447	A
32	1a	1456	G
32	1a	1487	G
32	1a	1492	A
32	1a	1493	A
32	1a	1497	G
32	1a	1503	A
32	1a	1504	G
32	1a	1506	U
32	1a	1517	G
32	1a	1529	G
32	1a	1530	G
32	1a	1532	U
53	1v	13	A
54	1w	2	C
54	1w	6	G
54	1w	8	4SU
54	1w	14	A
54	1w	19	G
54	1w	20	U
54	1w	21	A
54	1w	23	A
54	1w	24	G
54	1w	45	U
54	1w	46	7MG
54	1w	47	U
54	1w	48	C
54	1w	50	U
54	1w	62	C
54	1w	64	A
54	1w	68	C
54	1w	69	G
54	1w	70	G
54	1w	73	A
54	1w	74	C
55	1x	6	G
55	1x	9	G
55	1x	14	A
55	1x	18	G

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Mol	Chain	Res	Type
55	1x	21	A
55	1x	47	U
55	1x	61	C
55	1x	69	C
55	1x	76	A
54	1y	5	G
54	1y	6	G
54	1y	8	4SU
54	1y	9	A
54	1y	13	C
54	1y	19	G
54	1y	20	U
54	1y	21	A
54	1y	23	A
54	1y	35	A
54	1y	44	G
54	1y	45	U
54	1y	46	7MG
54	1y	47	U
54	1y	48	C
54	1y	49	C
54	1y	53	G
54	1y	54	5MU
54	1y	56	C
54	1y	59	U
54	1y	61	C
54	1y	65	G
54	1y	69	G
54	1y	70	G
1	2A	12	U
1	2A	15	G
1	2A	35	G
1	2A	36	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	94	C

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Mol	Chain	Res	Type
1	2A	95	G
1	2A	100	G
1	2A	102	G
1	2A	118	A
1	2A	119	A
1	2A	120	U
1	2A	125	G
1	2A	131	G
1	2A	154(A)	C
1	2A	157	U
1	2A	181	A
1	2A	196	A
1	2A	199	A
1	2A	205	G
1	2A	214	G
1	2A	215	G
1	2A	216	A
1	2A	221	A
1	2A	222	A
1	2A	226	G
1	2A	228	A
1	2A	229	A
1	2A	232	G
1	2A	233	A
1	2A	248	G
1	2A	249	C
1	2A	250	G
1	2A	271(J)	C
1	2A	271(K)	U
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	271(O)	C
1	2A	272(B)	G
1	2A	272(I)	U
1	2A	272(J)	C
1	2A	274	G
1	2A	277	C
1	2A	278	A
1	2A	280	C
1	2A	294	A
1	2A	303	U

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Mol	Chain	Res	Type
1	2A	311	A
1	2A	317	G
1	2A	324	A
1	2A	329	G
1	2A	330	A
1	2A	342	G
1	2A	352	G
1	2A	362	U
1	2A	363	G
1	2A	363(B)	G
1	2A	363(D)	G
1	2A	386	G
1	2A	396	G
1	2A	405	U
1	2A	406	G
1	2A	411	G
1	2A	412	A
1	2A	422	A
1	2A	435	C
1	2A	444	C
1	2A	454	A
1	2A	455	C
1	2A	456	C
1	2A	457	A
1	2A	459	U
1	2A	481	G
1	2A	498	G
1	2A	501	A
1	2A	504	U
1	2A	505	A
1	2A	509	C
1	2A	528	A
1	2A	529	A
1	2A	531	C
1	2A	532	A
1	2A	533	G
1	2A	563	G
1	2A	568	U
1	2A	573	G
1	2A	575	A
1	2A	599	G
1	2A	603	A

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Mol	Chain	Res	Type
1	2A	604	G
1	2A	607	U
1	2A	614(A)	U
1	2A	614(B)	G
1	2A	615	G
1	2A	616	G
1	2A	627	A
1	2A	637	A
1	2A	645	C
1	2A	651	G
1	2A	652(B)	A
1	2A	669	G
1	2A	686	G
1	2A	709	U
1	2A	717	G
1	2A	726	G
1	2A	730	C
1	2A	752	A
1	2A	753	C
1	2A	764	A
1	2A	771	G
1	2A	774	A
1	2A	775	G
1	2A	776	G
1	2A	782	A
1	2A	784	A
1	2A	785	G
1	2A	792	G
1	2A	805	G
1	2A	812	C
1	2A	819	A
1	2A	827	U
1	2A	857	C
1	2A	859	G
1	2A	866	A
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

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Mol	Chain	Res	Type
1	2A	884	C
1	2A	886	C
1	2A	887	A
1	2A	888	C
1	2A	889	C
1	2A	893	C
1	2A	894	C
1	2A	896	A
1	2A	900	A
1	2A	901	A
1	2A	910	A
1	2A	914	C
1	2A	915	C
1	2A	917	A
1	2A	932	G
1	2A	933	A
1	2A	941	A
1	2A	944	G
1	2A	945	A
1	2A	946	G
1	2A	953	A
1	2A	958	U
1	2A	959	A
1	2A	961	C
1	2A	974	G
1	2A	975	C
1	2A	982	C
1	2A	983	A
1	2A	990	A
1	2A	996	A
1	2A	997	G
1	2A	998	C
1	2A	1005	C
1	2A	1012	U
1	2A	1013	C
1	2A	1017	G
1	2A	1020	A
1	2A	1022	G
1	2A	1025	G
1	2A	1026	U
1	2A	1033	U
1	2A	1038	C

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Mol	Chain	Res	Type
1	2A	1039	G
1	2A	1041	C
1	2A	1043	C
1	2A	1114	G
1	2A	1116	C
1	2A	1129	A
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1139	G
1	2A	1142(A)	A
1	2A	1169	G
1	2A	1170	G
1	2A	1171	G
1	2A	1210	A
1	2A	1211	U
1	2A	1212	G
1	2A	1220	A
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	1306	C
1	2A	1314	C
1	2A	1352	U
1	2A	1359	A
1	2A	1360	A
1	2A	1365	A
1	2A	1368	G
1	2A	1370	C
1	2A	1384	A
1	2A	1385	G
1	2A	1386	C
1	2A	1411	C
1	2A	1416	G
1	2A	1417	C

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Mol	Chain	Res	Type
1	2A	1420	U
1	2A	1421	G
1	2A	1427	A
1	2A	1428	C
1	2A	1435	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	1482	G
1	2A	1490	A
1	2A	1493	C
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	1531	C
1	2A	1532	C
1	2A	1541	G
1	2A	1543	C
1	2A	1547	C
1	2A	1558	A
1	2A	1559	G
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1580	A
1	2A	1582	C
1	2A	1584	C
1	2A	1586	A
1	2A	1608	A
1	2A	1609	A
1	2A	1610	A
1	2A	1616	A
1	2A	1639	U
1	2A	1640	C

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Mol	Chain	Res	Type
1	2A	1648	C
1	2A	1654	A
1	2A	1663	C
1	2A	1664	A
1	2A	1669	A
1	2A	1670	C
1	2A	1674	G
1	2A	1696	G
1	2A	1700	A
1	2A	1701	A
1	2A	1703	G
1	2A	1721	G
1	2A	1722	A
1	2A	1739	U
1	2A	1740	G
1	2A	1746	G
1	2A	1756	G
1	2A	1758	G
1	2A	1762	A
1	2A	1763	G
1	2A	1764	G
1	2A	1773	A
1	2A	1780	A
1	2A	1782	C
1	2A	1786	A
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1812	A
1	2A	1816	G
1	2A	1819	A
1	2A	1835	G
1	2A	1839	G
1	2A	1847	A
1	2A	1848	A
1	2A	1877	A
1	2A	1878	G
1	2A	1896	G
1	2A	1900	A
1	2A	1906	G
1	2A	1913	A
1	2A	1914	C

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Mol	Chain	Res	Type
1	2A	1929	G
1	2A	1930	G
1	2A	1936	A
1	2A	1937	A
1	2A	1938	A
1	2A	1955	U
1	2A	1963	U
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1981	A
1	2A	1983	C
1	2A	1984	G
1	2A	1993	U
1	2A	1996	C
1	2A	1997	G
1	2A	2020	A
1	2A	2023	G
1	2A	2027	G
1	2A	2031	A
1	2A	2032	G
1	2A	2033	A
1	2A	2043	C
1	2A	2055	C
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G
1	2A	2062	A
1	2A	2069	G
1	2A	2096	U
1	2A	2105	C
1	2A	2110	G
1	2A	2111	C
1	2A	2112	G
1	2A	2116	G
1	2A	2119	A
1	2A	2120	G
1	2A	2122	U
1	2A	2124	G
1	2A	2126	A
1	2A	2127	G

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Mol	Chain	Res	Type
1	2A	2129	C
1	2A	2131	G
1	2A	2132	U
1	2A	2133	G
1	2A	2134	A
1	2A	2135	A
1	2A	2136	C
1	2A	2137	C
1	2A	2138	C
1	2A	2140	C
1	2A	2142	C
1	2A	2146	C
1	2A	2150	U
1	2A	2151	G
1	2A	2153	G
1	2A	2155	G
1	2A	2156	G
1	2A	2157	G
1	2A	2158	A
1	2A	2159	G
1	2A	2161	C
1	2A	2166	G
1	2A	2167	U
1	2A	2168	G
1	2A	2172	U
1	2A	2174	C
1	2A	2178	C
1	2A	2182	G
1	2A	2185	C
1	2A	2189	U
1	2A	2192	G
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2218	U
1	2A	2225	A
1	2A	2236	C
1	2A	2238	G
1	2A	2239	G
1	2A	2275	C
1	2A	2279	G

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Mol	Chain	Res	Type
1	2A	2283	C
1	2A	2287	A
1	2A	2288	A
1	2A	2304	G
1	2A	2305	A
1	2A	2308	G
1	2A	2309	A
1	2A	2311	A
1	2A	2319	G
1	2A	2320	A
1	2A	2321	G
1	2A	2322	A
1	2A	2325	G
1	2A	2327	A
1	2A	2334	G
1	2A	2336	A
1	2A	2346	A
1	2A	2347	C
1	2A	2350	C
1	2A	2372	G
1	2A	2376	A
1	2A	2383	G
1	2A	2385	C
1	2A	2402	C
1	2A	2403	C
1	2A	2406	U
1	2A	2410	G
1	2A	2413	G
1	2A	2425	A
1	2A	2428	G
1	2A	2429	G
1	2A	2430	A
1	2A	2434	A
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2448	A
1	2A	2474	C
1	2A	2476	A
1	2A	2477	C
1	2A	2491	U
1	2A	2494	G

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Mol	Chain	Res	Type
1	2A	2502	G
1	2A	2505	G
1	2A	2506	U
1	2A	2518	A
1	2A	2520	C
1	2A	2525	G
1	2A	2529	G
1	2A	2541	A
1	2A	2549	G
1	2A	2554	U
1	2A	2555	U
1	2A	2566	A
1	2A	2567	G
1	2A	2574	G
1	2A	2578	G
1	2A	2585	U
1	2A	2592	G
1	2A	2602	A
1	2A	2609	U
1	2A	2611	U
1	2A	2612	C
1	2A	2630	G
1	2A	2634	G
1	2A	2654	A
1	2A	2669	G
1	2A	2689	U
1	2A	2690	C
1	2A	2702	U
1	2A	2703	C
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G
1	2A	2726	U
1	2A	2733	A
1	2A	2748	A
1	2A	2751	G
1	2A	2761	G
1	2A	2764	A
1	2A	2765	A
1	2A	2778	A
1	2A	2779	U
1	2A	2780	G

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Mol	Chain	Res	Type
1	2A	2793	G
1	2A	2794	C
1	2A	2802	G
1	2A	2807	G
1	2A	2818	G
1	2A	2820	A
1	2A	2821	A
1	2A	2833	G
1	2A	2834	G
1	2A	2835	A
1	2A	2837	G
1	2A	2839	G
1	2A	2872	G
1	2A	2873	A
1	2A	2879	C
1	2A	2880	C
1	2A	2894	G
1	2A	2897	U
2	2B	2	C
2	2B	5	C
2	2B	7	G
2	2B	8	U
2	2B	9	G
2	2B	13	A
2	2B	19	G
2	2B	20	C
2	2B	25	A
2	2B	30	C
2	2B	31	C
2	2B	34	U
2	2B	42	C
2	2B	53	A
2	2B	56	G
2	2B	58	A
2	2B	65	C
2	2B	66	A
2	2B	67	G
2	2B	69	G
2	2B	72	G
2	2B	73	A
2	2B	74	U
2	2B	75	G

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Mol	Chain	Res	Type
2	2B	85	G
2	2B	88	C
2	2B	106	G
2	2B	108	U
2	2B	110	G
2	2B	114	C
2	2B	116	G
2	2B	119	G
2	2B	120	A
32	2a	9	G
32	2a	22	G
32	2a	31	G
32	2a	32	A
32	2a	39	G
32	2a	44	G
32	2a	47	C
32	2a	48	C
32	2a	50	A
32	2a	51	A
32	2a	54	C
32	2a	66	G
32	2a	73	G
32	2a	80	G
32	2a	88	A
32	2a	89	C
32	2a	98	G
32	2a	101	A
32	2a	105	G
32	2a	116	A
32	2a	120	A
32	2a	121	C
32	2a	131	C
32	2a	144	G
32	2a	163	C
32	2a	174	C
32	2a	180	U
32	2a	182	U
32	2a	184	G
32	2a	188	C
32	2a	189(A)	C
32	2a	189(F)	U
32	2a	189(G)	G

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Mol	Chain	Res	Type
32	2a	195	A
32	2a	197	A
32	2a	201	C
32	2a	202	U
32	2a	203	U
32	2a	204	U
32	2a	216	G
32	2a	247	G
32	2a	251	G
32	2a	258	G
32	2a	266	G
32	2a	267	C
32	2a	281	G
32	2a	289	G
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	350	G
32	2a	351	G
32	2a	352	C
32	2a	353	A
32	2a	354	G
32	2a	367	U
32	2a	372	C
32	2a	384	G
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	412	A
32	2a	414	A
32	2a	421	U
32	2a	423	G
32	2a	424	G
32	2a	429	U
32	2a	430	A
32	2a	442	C
32	2a	452	A
32	2a	461	A
32	2a	470	C
32	2a	471	G
32	2a	484	G
32	2a	485	G

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Mol	Chain	Res	Type
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	521	G
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	572	A
32	2a	573	A
32	2a	576	G
32	2a	577	G
32	2a	596	C
32	2a	601	C
32	2a	619	U
32	2a	630	G
32	2a	650	G
32	2a	653	A
32	2a	665	A
32	2a	671	G
32	2a	672	U
32	2a	687	A
32	2a	688	G
32	2a	695	A
32	2a	702	A
32	2a	703	G
32	2a	708	C
32	2a	720	C
32	2a	721	G
32	2a	723	U
32	2a	724	G
32	2a	731	G
32	2a	734	G
32	2a	749	C

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Mol	Chain	Res	Type
32	2a	755	G
32	2a	777	A
32	2a	792	A
32	2a	793	U
32	2a	794	A
32	2a	805	C
32	2a	816	A
32	2a	817	C
32	2a	821	G
32	2a	828	A
32	2a	834	C
32	2a	840	C
32	2a	841	U
32	2a	859	A
32	2a	884	U
32	2a	885	G
32	2a	902	G
32	2a	914	A
32	2a	926	G
32	2a	927	G
32	2a	934	C
32	2a	935	A
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	982	U
32	2a	989	C
32	2a	992	U
32	2a	993	G
32	2a	995	C
32	2a	996	A
32	2a	997	U
32	2a	999	C
32	2a	1001	A
32	2a	1001(A)	G

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Mol	Chain	Res	Type
32	2a	1002	G
32	2a	1003	G
32	2a	1004	A
32	2a	1005	A
32	2a	1006	C
32	2a	1007	C
32	2a	1009	G
32	2a	1011	G
32	2a	1020	U
32	2a	1021	G
32	2a	1022	G
32	2a	1025	U
32	2a	1026	G
32	2a	1027	C
32	2a	1029	C
32	2a	1030(A)	G
32	2a	1031	G
32	2a	1032	G
32	2a	1033	G
32	2a	1035	A
32	2a	1036	G
32	2a	1038	C
32	2a	1039	C
32	2a	1040	U
32	2a	1045	C
32	2a	1051	C
32	2a	1054	C
32	2a	1055	A
32	2a	1056	U
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1071	C
32	2a	1077	G
32	2a	1081	G
32	2a	1086	U
32	2a	1087	G
32	2a	1094	G
32	2a	1095	U
32	2a	1101	A
32	2a	1113	C
32	2a	1117	G

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Mol	Chain	Res	Type
32	2a	1121	U
32	2a	1122	U
32	2a	1125	U
32	2a	1129	C
32	2a	1130	A
32	2a	1132	C
32	2a	1136	U
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G
32	2a	1140	C
32	2a	1143	G
32	2a	1146	A
32	2a	1152	A
32	2a	1157	A
32	2a	1158	C
32	2a	1159	U
32	2a	1172	C
32	2a	1174	G
32	2a	1182	G
32	2a	1183	A
32	2a	1184	G
32	2a	1196	U
32	2a	1197	G
32	2a	1200	C
32	2a	1201	A
32	2a	1202	G
32	2a	1211	U
32	2a	1212	U
32	2a	1213	A
32	2a	1214	C
32	2a	1227	A
32	2a	1238	A
32	2a	1240	U
32	2a	1241	G
32	2a	1246	C
32	2a	1256	A
32	2a	1257	U
32	2a	1258	G
32	2a	1260	C
32	2a	1261	A
32	2a	1267	C

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Mol	Chain	Res	Type
32	2a	1270	C
32	2a	1272	G
32	2a	1273	G
32	2a	1276	G
32	2a	1277	C
32	2a	1278	U
32	2a	1279	A
32	2a	1280	A
32	2a	1287	A
32	2a	1301	U
32	2a	1302	U
32	2a	1303	C
32	2a	1305	G
32	2a	1319	A
32	2a	1338	G
32	2a	1340	A
32	2a	1346	A
32	2a	1347	G
32	2a	1349	A
32	2a	1358	U
32	2a	1363	C
32	2a	1368	G
32	2a	1370	G
32	2a	1388	C
32	2a	1400	5MC
32	2a	1404	5MC
32	2a	1406	U
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1446	U
32	2a	1447	A
32	2a	1452	C
32	2a	1456	G
32	2a	1492	A
32	2a	1499	A
32	2a	1503	A
32	2a	1504	G
32	2a	1506	U
32	2a	1517	G
32	2a	1520	G
32	2a	1529	G

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Mol	Chain	Res	Type
32	2a	1530	G
32	2a	1531	A
32	2a	1532	U
53	2v	13	A
53	2v	14	A
53	2v	15	A
53	2v	24	A
54	2w	3	C
54	2w	4	C
54	2w	5	G
54	2w	7	A
54	2w	9	A
54	2w	11	C
54	2w	13	C
54	2w	14	A
54	2w	19	G
54	2w	22	G
54	2w	29	G
54	2w	34	G
54	2w	40	C
54	2w	46	7MG
54	2w	47	U
54	2w	48	C
54	2w	50	U
54	2w	56	C
54	2w	62	C
54	2w	63	G
54	2w	64	A
54	2w	68	C
54	2w	69	G
54	2w	74	C
55	2x	9	G
55	2x	13	C
55	2x	18	G
55	2x	21	A
55	2x	42	G
55	2x	43	A
55	2x	47	U
55	2x	48	C
55	2x	52	G
55	2x	53	G
55	2x	65	C

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Mol	Chain	Res	Type
55	2x	67	C
55	2x	68	C
55	2x	76	A
54	2y	15	G
54	2y	19	G
54	2y	23	A
54	2y	24	G
54	2y	25	C
54	2y	27	G
54	2y	34	G
54	2y	45	U
54	2y	49	C
54	2y	52	G
54	2y	53	G
54	2y	55	PSU
54	2y	56	C
54	2y	57	G
54	2y	58	A
54	2y	59	U
54	2y	61	C
54	2y	62	C
54	2y	63	G
54	2y	65	G
54	2y	69	G
54	2y	70	G
54	2y	73	A

All (53) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	115	G
1	1A	184	A
1	1A	271	U
1	1A	302	A
1	1A	509	A
1	1A	572	A
1	1A	913	A
1	1A	941	U
1	1A	1065	U
1	1A	1067	A
1	1A	1093	G
1	1A	1124	U

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Mol	Chain	Res	Type
1	1A	1201	A
1	1A	1219	A
1	1A	1220	U
1	1A	1221	G
1	1A	1466	U
1	1A	1554	A
1	1A	1654	A
1	1A	2014	G
1	1A	2156	A
1	1A	2180	A
1	1A	2192	A
1	1A	2203	G
1	1A	2205	C
1	1A	2418	U
1	1A	2442	A
1	1A	2641	A
1	1A	2701	U
2	1B	1	U
1	2A	34	C
1	2A	195	A
1	2A	228	A
1	2A	266	G
1	2A	271(K)	U
1	2A	271(M)	G
1	2A	277	C
1	2A	528	A
1	2A	752	A
1	2A	827	U
1	2A	856	C
1	2A	900	A
1	2A	1210	A
1	2A	1420	U
1	2A	1442	G
1	2A	1530	C
1	2A	1653	G
1	2A	1695	G
1	2A	1913	A
1	2A	1992	G
1	2A	2119	A
1	2A	2126	A
1	2A	2689	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	$\#\|Z\| > 2$
54	5MU	1w	54	54	19,22,23	1.48	4 (21%)	28,32,35	1.83	6 (21%)
54	4SU	1y	8	54	18,21,22	1.63	4 (22%)	26,30,33	1.85	5 (19%)
32	MA6	1a	1519	32	19,26,27	1.02	1 (5%)	18,38,41	1.65	4 (22%)
55	5MC	2x	32	55	18,22,23	1.04	1 (5%)	26,32,35	1.15	3 (11%)
32	2MG	2a	1207	32	18,26,27	0.92	1 (5%)	16,38,41	1.10	1 (6%)
1	5MU	1A	1961	56,1	19,22,23	1.36	4 (21%)	28,32,35	2.19	6 (21%)
32	2MG	1a	1207	32	18,26,27	0.96	1 (5%)	16,38,41	1.10	2 (12%)
32	4OC	2a	1402	56,32	20,23,24	0.78	0	26,32,35	1.16	2 (7%)
54	4SU	2w	8	54	18,21,22	1.65	4 (22%)	26,30,33	2.29	5 (19%)
55	PSU	1x	55	55	18,21,22	1.28	2 (11%)	22,30,33	1.86	4 (18%)
32	MA6	2a	1518	32	19,26,27	1.00	1 (5%)	18,38,41	1.64	5 (27%)
1	5MC	2A	1962	56,1	18,22,23	0.93	2 (11%)	26,32,35	1.21	2 (7%)
32	MA6	2a	1519	32	19,26,27	1.00	1 (5%)	18,38,41	1.60	4 (22%)
54	PSU	1y	39	54	18,21,22	1.39	2 (11%)	22,30,33	1.72	3 (13%)
54	PSU	1y	55	54	18,21,22	1.31	2 (11%)	22,30,33	1.95	4 (18%)
1	2MU	2A	2552	56,1	19,22,24	1.22	2 (10%)	26,31,36	1.85	5 (19%)
54	7MG	2y	46	54	22,26,27	1.48	4 (18%)	29,39,42	2.67	7 (24%)
1	5MC	1A	1984	1	18,22,23	0.91	2 (11%)	26,32,35	1.23	2 (7%)
54	4SU	1w	8	54	18,21,22	1.62	4 (22%)	26,30,33	2.05	4 (15%)
32	MA6	1a	1518	32	19,26,27	0.95	1 (5%)	18,38,41	1.69	5 (27%)
32	5MC	1a	967	32	18,22,23	0.95	2 (11%)	26,32,35	1.17	2 (7%)
1	5MU	2A	1939	1	19,22,23	1.43	5 (26%)	28,32,35	2.36	6 (21%)
54	PSU	1w	39	54	18,21,22	1.33	2 (11%)	22,30,33	1.81	3 (13%)
32	UR3	1a	1498	32	19,22,23	1.09	1 (5%)	26,32,35	1.52	2 (7%)
55	4SU	1x	8	55	18,21,22	2.03	4 (22%)	26,30,33	1.41	5 (19%)
32	5MC	2a	967	32	18,22,23	0.99	2 (11%)	26,32,35	1.19	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
55	5MU	2x	54	55	19,22,23	1.42	5 (26%)	28,32,35	2.27	6 (21%)
54	7MG	1y	46	54	22,26,27	1.35	4 (18%)	29,39,42	2.48	6 (20%)
32	5MC	1a	1400	32	18,22,23	0.97	2 (11%)	26,32,35	1.20	3 (11%)
54	4SU	2y	8	54	18,21,22	1.78	4 (22%)	26,30,33	2.20	5 (19%)
1	PSU	1A	1939	1	18,21,22	1.43	4 (22%)	22,30,33	1.91	3 (13%)
54	PSU	2y	32	54	18,21,22	1.31	2 (11%)	22,30,33	1.79	4 (18%)
1	2MA	1A	2515	56,1	17,25,26	0.99	1 (5%)	17,37,40	1.01	2 (11%)
1	5MU	1A	1937	1	19,22,23	1.38	6 (31%)	28,32,35	2.21	6 (21%)
1	PSU	1A	2617	1	18,21,22	1.38	4 (22%)	22,30,33	1.81	4 (18%)
32	5MC	2a	1400	32	18,22,23	0.95	2 (11%)	26,32,35	1.10	2 (7%)
1	2MA	2A	2503	56,1	17,25,26	0.97	1 (5%)	17,37,40	1.05	2 (11%)
1	OMG	1A	2263	56,55,1	18,26,27	1.00	1 (5%)	19,38,41	1.07	2 (10%)
32	5MC	1a	1407	32	18,22,23	0.93	2 (11%)	26,32,35	1.19	2 (7%)
1	4OC	2A	1920	1	19,22,24	0.81	0	26,31,35	0.83	0
32	M2G	1a	966	32	20,27,28	1.42	3 (15%)	22,40,43	0.97	2 (9%)
55	5MC	1x	32	55	18,22,23	1.05	2 (11%)	26,32,35	1.11	3 (11%)
54	PSU	2w	39	54	18,21,22	1.40	2 (11%)	22,30,33	1.61	4 (18%)
54	5MU	1y	54	54	19,22,23	1.57	6 (31%)	28,32,35	1.97	6 (21%)
32	5MC	2a	1407	32	18,22,23	1.00	2 (11%)	26,32,35	1.25	3 (11%)
54	MIA	1y	37	54	18,24,32	1.14	2 (11%)	18,35,47	1.34	2 (11%)
54	PSU	2w	55	54	18,21,22	1.35	2 (11%)	22,30,33	1.98	4 (18%)
54	7MG	1w	46	54	22,26,27	1.44	4 (18%)	29,39,42	2.40	6 (20%)
32	4OC	1a	1402	56,32	20,23,24	0.75	0	26,32,35	0.91	1 (3%)
54	PSU	1y	32	54	18,21,22	1.38	3 (16%)	22,30,33	1.74	3 (13%)
54	PSU	1w	55	54	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
54	MIA	2w	37	54	20,27,32	1.83	3 (15%)	22,39,47	1.87	8 (36%)
55	PSU	2x	55	55	18,21,22	1.33	2 (11%)	22,30,33	1.84	4 (18%)
54	5MU	2y	54	54	19,22,23	1.50	4 (21%)	28,32,35	2.10	9 (32%)
43	0TD	1l	92	43	7,9,10	4.82	1 (14%)	6,11,13	3.69	3 (50%)
1	PSU	2A	1917	56,1	18,21,22	1.39	2 (11%)	22,30,33	1.93	3 (13%)
32	M2G	2a	966	32	20,27,28	1.49	3 (15%)	22,40,43	0.91	2 (9%)
32	5MC	1a	1404	56,32	18,22,23	1.00	2 (11%)	26,32,35	1.09	3 (11%)
54	PSU	1w	32	54	18,21,22	1.34	2 (11%)	22,30,33	1.82	3 (13%)
1	PSU	2A	2605	1	18,21,22	1.33	3 (16%)	22,30,33	1.96	3 (13%)
1	OMG	2A	2251	55,1	18,26,27	1.05	1 (5%)	19,38,41	1.13	3 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	7MG	2a	527	32	22,26,27	1.37	3 (13%)	29,39,42	2.51	7 (24%)
1	2MU	1A	2564	56,1	19,22,24	1.18	2 (10%)	26,31,36	2.04	6 (23%)
32	PSU	2a	516	32	18,21,22	1.33	2 (11%)	22,30,33	1.78	4 (18%)
32	PSU	1a	516	56,32	18,21,22	1.31	2 (11%)	22,30,33	1.88	5 (22%)
1	PSU	1A	1933	1	18,21,22	1.38	2 (11%)	22,30,33	1.99	3 (13%)
1	PSU	2A	1911	1	18,21,22	1.37	2 (11%)	22,30,33	1.80	3 (13%)
54	7MG	2w	46	54	22,26,27	1.35	5 (22%)	29,39,42	2.55	7 (24%)
32	5MC	2a	1404	32	18,22,23	0.98	2 (11%)	26,32,35	1.19	2 (7%)
43	0TD	2l	92	43	7,9,10	4.72	1 (14%)	6,11,13	1.73	2 (33%)
1	5MC	1A	1964	1	18,22,23	0.95	2 (11%)	26,32,35	1.17	3 (11%)
32	7MG	1a	527	32	22,26,27	1.46	4 (18%)	29,39,42	2.46	6 (20%)
54	MIA	1w	37	54	24,31,32	2.32	4 (16%)	26,44,47	2.68	10 (38%)
32	UR3	2a	1498	32	19,22,23	1.06	1 (5%)	26,32,35	1.51	2 (7%)
54	PSU	2y	39	54	18,21,22	1.34	2 (11%)	22,30,33	1.78	3 (13%)
55	4SU	2x	8	55,56	18,21,22	1.89	5 (27%)	26,30,33	1.40	4 (15%)
1	5MC	2A	1942	1	18,22,23	0.95	2 (11%)	26,32,35	1.08	2 (7%)
54	PSU	2y	55	54	18,21,22	1.29	3 (16%)	22,30,33	1.77	5 (22%)
54	5MU	2w	54	54	19,22,23	1.34	4 (21%)	28,32,35	1.80	6 (21%)
1	5MU	2A	1915	1	19,22,23	1.52	5 (26%)	28,32,35	2.12	7 (25%)
54	MIA	2y	37	54,32	18,24,32	1.11	2 (11%)	18,35,47	1.33	3 (16%)
1	4OC	1A	1942	56,1	19,22,24	0.82	0	26,31,35	0.86	0
54	PSU	2w	32	54	18,21,22	1.34	2 (11%)	22,30,33	1.79	3 (13%)
55	5MU	1x	54	55	19,22,23	1.43	5 (26%)	28,32,35	1.89	7 (25%)

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
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
54	4SU	1y	8	54	-	3/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	3/7/29/30	0/3/3/3
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	1/5/27/28	0/3/3/3
1	5MU	1A	1961	56,1	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	4OC	2a	1402	56,32	-	3/9/29/30	0/2/2/2
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2
55	PSU	1x	55	55	-	2/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	2/7/29/30	0/3/3/3
1	5MC	2A	1962	56,1	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	4/7/29/30	0/3/3/3
54	PSU	1y	39	54	-	0/7/25/26	0/2/2/2
54	PSU	1y	55	54	-	1/7/25/26	0/2/2/2
1	2MU	2A	2552	56,1	-	1/9/27/28	0/2/2/2
54	7MG	2y	46	54	-	3/7/37/38	0/3/3/3
1	5MC	1A	1984	1	-	0/7/25/26	0/2/2/2
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	1/7/29/30	0/3/3/3
32	5MC	1a	967	32	-	1/7/25/26	0/2/2/2
1	5MU	2A	1939	1	-	0/7/25/26	0/2/2/2
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	2/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
54	7MG	1y	46	54	-	2/7/37/38	0/3/3/3
32	5MC	1a	1400	32	-	2/7/25/26	0/2/2/2
54	4SU	2y	8	54	-	1/7/25/26	0/2/2/2
1	PSU	1A	1939	1	-	0/7/25/26	0/2/2/2
54	PSU	2y	32	54	-	2/7/25/26	0/2/2/2
1	2MA	1A	2515	56,1	-	2/3/25/26	0/3/3/3
1	5MU	1A	1937	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	2617	1	-	0/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	56,1	-	1/3/25/26	0/3/3/3
1	OMG	1A	2263	56,55,1	-	1/5/27/28	0/3/3/3
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
1	4OC	2A	1920	1	-	0/9/27/30	0/2/2/2
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
54	5MU	1y	54	54	-	3/7/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
54	MIA	1y	37	54	-	0/3/25/34	0/3/3/3
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	7MG	1w	46	54	-	3/7/37/38	0/3/3/3
32	4OC	1a	1402	56,32	-	0/9/29/30	0/2/2/2
54	PSU	1y	32	54	-	0/7/25/26	0/2/2/2
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
54	MIA	2w	37	54	-	1/7/29/34	0/3/3/3
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
54	5MU	2y	54	54	-	2/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	2/7/12/14	-
1	PSU	2A	1917	56,1	-	2/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
32	5MC	1a	1404	56,32	-	0/7/25/26	0/2/2/2
54	PSU	1w	32	54	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	55,1	-	0/5/27/28	0/3/3/3
32	7MG	2a	527	32	-	3/7/37/38	0/3/3/3
1	2MU	1A	2564	56,1	-	0/9/27/28	0/2/2/2
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	56,32	-	0/7/25/26	0/2/2/2
1	PSU	1A	1933	1	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
54	7MG	2w	46	54	-	4/7/37/38	0/3/3/3
32	5MC	2a	1404	32	-	1/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	1/7/12/14	-
1	5MC	1A	1964	1	-	0/7/25/26	0/2/2/2
32	7MG	1a	527	32	-	3/7/37/38	0/3/3/3
54	MIA	1w	37	54	-	1/11/33/34	0/3/3/3
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
54	PSU	2y	39	54	-	0/7/25/26	0/2/2/2
55	4SU	2x	8	55,56	-	1/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
54	PSU	2y	55	54	-	3/7/25/26	0/2/2/2
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
54	MIA	2y	37	54,32	-	3/3/25/34	0/3/3/3
1	4OC	1A	1942	56,1	-	1/9/27/30	0/2/2/2
54	PSU	2w	32	54	-	0/7/25/26	0/2/2/2
55	5MU	1x	54	55	-	0/7/25/26	0/2/2/2

All (210) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-12.41	1.69	1.82
43	2l	92	0TD	CB-SB	-12.19	1.69	1.82
54	1w	37	MIA	C2-S10	-7.64	1.69	1.75
54	1w	37	MIA	C13-C14	7.02	1.52	1.32
54	2w	37	MIA	C2-S10	-6.89	1.69	1.75
32	2a	966	M2G	C2-N3	4.85	1.36	1.30
55	1x	8	4SU	C4-N3	-4.64	1.32	1.37
54	2y	8	4SU	C4-S4	-4.51	1.59	1.68
32	1a	966	M2G	C2-N3	4.36	1.36	1.30
54	2w	8	4SU	C4-S4	-4.35	1.60	1.68
55	2x	8	4SU	C4-N3	-4.21	1.33	1.37
55	1x	8	4SU	C4-S4	-4.06	1.60	1.68
54	1w	8	4SU	C4-S4	-3.99	1.60	1.68
55	2x	8	4SU	C4-S4	-3.98	1.60	1.68
54	1y	32	PSU	C6-C5	3.92	1.39	1.35
54	1y	8	4SU	C4-S4	-3.87	1.61	1.68
54	1y	39	PSU	C6-C5	3.78	1.39	1.35
54	2w	39	PSU	C6-C5	3.78	1.39	1.35
55	1x	8	4SU	C2-N3	-3.75	1.31	1.38
54	1w	55	PSU	C6-C5	3.74	1.39	1.35
54	2w	55	PSU	C6-C5	3.71	1.39	1.35
55	2x	55	PSU	C6-C5	3.61	1.39	1.35
54	2y	32	PSU	C6-C5	3.52	1.39	1.35
54	1w	39	PSU	C6-C5	3.51	1.39	1.35
54	1w	46	7MG	C4-N9	-3.48	1.33	1.37
32	2a	516	PSU	C6-C5	3.43	1.39	1.35
54	2y	39	PSU	C6-C5	3.43	1.39	1.35
54	1w	32	PSU	C6-C5	3.42	1.39	1.35
54	2y	46	7MG	C5-C4	3.40	1.49	1.38
32	1a	527	7MG	C4-N9	-3.40	1.33	1.37
32	2a	527	7MG	C4-N9	-3.37	1.33	1.37
1	2A	1911	PSU	C6-C5	3.37	1.39	1.35
54	2y	54	5MU	C2-N1	3.34	1.43	1.38
54	1y	55	PSU	C6-C5	3.34	1.39	1.35
1	1A	1933	PSU	C6-C5	3.33	1.39	1.35
54	2w	32	PSU	C6-C5	3.28	1.39	1.35
54	1y	8	4SU	C4-N3	-3.26	1.34	1.37
55	2x	8	4SU	C2-N3	-3.22	1.32	1.38
54	1y	54	5MU	C6-C5	3.17	1.39	1.34
54	1w	46	7MG	C5-C4	3.14	1.48	1.38
54	1y	46	7MG	C5-C4	3.12	1.48	1.38
32	1a	516	PSU	C6-C5	3.12	1.39	1.35
55	2x	32	5MC	C6-C5	3.10	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2y	46	7MG	C8-N9	3.09	1.47	1.46
32	1a	527	7MG	C5-C4	3.08	1.48	1.38
54	2w	46	7MG	C5-C4	3.07	1.48	1.38
32	2a	1407	5MC	C6-C5	3.05	1.39	1.34
1	1A	1939	PSU	C6-C5	3.05	1.38	1.35
55	1x	32	5MC	C6-C5	3.05	1.39	1.34
55	1x	8	4SU	C5-C4	-3.05	1.38	1.42
1	2A	2251	OMG	C6-N1	-3.02	1.33	1.37
1	1A	2617	PSU	C6-C5	2.98	1.38	1.35
54	2y	8	4SU	C4-N3	-2.98	1.34	1.37
1	2A	1917	PSU	C6-C5	2.97	1.38	1.35
32	1a	966	M2G	C2-N2	2.96	1.40	1.35
54	1w	54	5MU	C6-C5	2.93	1.39	1.34
32	2a	527	7MG	C5-C4	2.92	1.47	1.38
55	1x	54	5MU	C6-C5	2.91	1.39	1.34
1	2A	1915	5MU	C2-N1	2.91	1.43	1.38
54	2w	46	7MG	C4-N9	-2.91	1.34	1.37
1	1A	1961	5MU	C4-N3	-2.89	1.33	1.38
1	2A	1915	5MU	C6-C5	2.89	1.39	1.34
54	1y	54	5MU	C2-N1	2.88	1.43	1.38
55	1x	55	PSU	C6-C5	2.88	1.38	1.35
1	2A	2605	PSU	C6-C5	2.87	1.38	1.35
32	2a	1404	5MC	C6-C5	2.84	1.39	1.34
55	2x	54	5MU	C6-C5	2.84	1.39	1.34
1	2A	1939	5MU	C4-N3	-2.83	1.33	1.38
32	2a	966	M2G	C2-N2	2.83	1.40	1.35
1	1A	2263	OMG	C6-N1	-2.83	1.33	1.37
1	1A	2564	2MU	C4-N3	-2.83	1.33	1.38
1	1A	2617	PSU	C4-N3	-2.81	1.33	1.38
32	2a	967	5MC	C6-C5	2.81	1.39	1.34
1	2A	1915	5MU	C4-C5	2.79	1.49	1.44
32	1a	1404	5MC	C6-C5	2.78	1.39	1.34
54	1w	54	5MU	C4-C5	2.78	1.49	1.44
1	2A	1939	5MU	C6-C5	2.78	1.39	1.34
54	2w	8	4SU	C4-N3	-2.78	1.34	1.37
1	1A	1937	5MU	C4-N3	-2.77	1.33	1.38
1	2A	1942	5MC	C6-C5	2.76	1.39	1.34
1	2A	1917	PSU	C4-N3	-2.75	1.33	1.38
55	2x	54	5MU	C4-C5	2.74	1.49	1.44
54	2y	8	4SU	C2-N1	2.73	1.42	1.38
32	2a	1518	MA6	C5-C4	2.73	1.48	1.40
54	1y	54	5MU	C4-N3	-2.71	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	8	4SU	C4-N3	-2.69	1.34	1.37
54	2w	39	PSU	C4-N3	-2.69	1.33	1.38
32	1a	967	5MC	C6-C5	2.68	1.39	1.34
54	1y	37	MIA	C5-C4	2.68	1.48	1.40
54	2y	37	MIA	C5-C4	2.67	1.48	1.40
1	1A	1939	PSU	C4-N3	-2.66	1.33	1.38
1	1A	1933	PSU	C4-N3	-2.64	1.33	1.38
1	2A	2605	PSU	C4-N3	-2.64	1.33	1.38
54	1y	39	PSU	C4-N3	-2.63	1.33	1.38
1	2A	1962	5MC	C6-N1	-2.63	1.33	1.38
32	2a	1400	5MC	C6-C5	2.62	1.38	1.34
32	2a	1519	MA6	C5-C4	2.61	1.47	1.40
1	1A	1984	5MC	C6-N1	-2.61	1.33	1.38
54	2y	54	5MU	C6-C5	2.60	1.38	1.34
55	1x	55	PSU	C4-N3	-2.60	1.34	1.38
1	2A	1915	5MU	C4-N3	-2.60	1.34	1.38
54	2y	8	4SU	C5-C4	-2.60	1.39	1.42
54	2y	55	PSU	C6-C5	2.59	1.38	1.35
32	1a	1400	5MC	C6-C5	2.59	1.38	1.34
54	1y	54	5MU	C4-C5	2.59	1.49	1.44
54	1y	37	MIA	C2-N3	2.58	1.36	1.32
1	1A	1964	5MC	C6-C5	2.57	1.38	1.34
54	1w	54	5MU	C4-N3	-2.57	1.34	1.38
54	2w	37	MIA	C5-C4	2.56	1.47	1.40
1	1A	1937	5MU	C6-C5	2.56	1.38	1.34
1	2A	1911	PSU	C4-N3	-2.56	1.34	1.38
1	2A	1939	5MU	C6-N1	-2.56	1.33	1.38
54	2y	54	5MU	C4-C5	2.55	1.49	1.44
54	2y	37	MIA	C2-N3	2.54	1.36	1.32
54	1w	32	PSU	C4-N3	-2.54	1.34	1.38
54	2y	46	7MG	C6-N1	-2.54	1.34	1.38
55	2x	8	4SU	C5-C4	-2.53	1.39	1.42
32	1a	527	7MG	C6-N1	-2.52	1.34	1.38
55	1x	54	5MU	C4-C5	2.52	1.49	1.44
55	1x	54	5MU	C4-N3	-2.51	1.34	1.38
54	2y	39	PSU	C4-N3	-2.51	1.34	1.38
54	1y	46	7MG	C8-N9	2.51	1.47	1.46
54	2w	55	PSU	C4-N3	-2.50	1.34	1.38
54	2w	54	5MU	C6-C5	2.50	1.38	1.34
54	1w	46	7MG	C6-N1	-2.49	1.34	1.38
1	1A	1961	5MU	C6-N1	-2.47	1.33	1.38
54	1w	55	PSU	C4-N3	-2.47	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1y	55	PSU	C4-N3	-2.47	1.34	1.38
32	1a	1519	MA6	C5-C4	2.47	1.47	1.40
32	1a	1400	5MC	C6-N1	-2.46	1.33	1.38
1	1A	1961	5MU	C6-C5	2.45	1.38	1.34
54	1w	37	MIA	C5-C4	2.43	1.47	1.40
55	2x	55	PSU	C4-N3	-2.43	1.34	1.38
54	1w	39	PSU	C4-N3	-2.43	1.34	1.38
54	1w	8	4SU	C2-N1	2.43	1.42	1.38
54	2w	8	4SU	C2-N1	2.42	1.42	1.38
32	2a	516	PSU	C4-N3	-2.42	1.34	1.38
1	1A	1964	5MC	C6-N1	-2.42	1.33	1.38
54	2y	55	PSU	C4-N3	-2.41	1.34	1.38
54	2y	54	5MU	C4-N3	-2.40	1.34	1.38
32	1a	1207	2MG	C6-N1	-2.40	1.34	1.37
55	1x	32	5MC	C6-N1	-2.40	1.34	1.38
1	1A	1961	5MU	C2-N3	-2.39	1.33	1.38
1	2A	2552	2MU	C5-C4	2.39	1.48	1.43
1	1A	1939	PSU	C2-N1	-2.39	1.33	1.36
54	1w	54	5MU	C2-N1	2.39	1.42	1.38
32	1a	516	PSU	C4-N3	-2.37	1.34	1.38
54	2w	32	PSU	C4-N3	-2.35	1.34	1.38
54	2y	32	PSU	C4-N3	-2.34	1.34	1.38
1	2A	1939	5MU	C4-C5	2.33	1.48	1.44
54	2w	54	5MU	C4-C5	2.33	1.48	1.44
32	1a	1407	5MC	C6-C5	2.33	1.38	1.34
32	1a	966	M2G	C6-N1	-2.32	1.34	1.37
32	2a	527	7MG	C6-N1	-2.32	1.34	1.38
32	1a	1404	5MC	C6-N1	-2.31	1.34	1.38
54	1y	8	4SU	C5-C4	-2.30	1.39	1.42
32	2a	966	M2G	C6-N1	-2.30	1.34	1.37
32	1a	1498	UR3	C2-N1	2.30	1.41	1.38
55	2x	54	5MU	C4-N3	-2.29	1.34	1.38
32	1a	1518	MA6	C5-C4	2.29	1.47	1.40
54	2w	54	5MU	C4-N3	-2.28	1.34	1.38
54	1w	8	4SU	C5-C4	-2.27	1.39	1.42
32	1a	1407	5MC	C6-N1	-2.27	1.34	1.38
1	2A	1962	5MC	C6-C5	2.26	1.38	1.34
54	2w	46	7MG	C8-N9	2.26	1.47	1.46
55	2x	54	5MU	C6-N1	-2.25	1.34	1.38
54	1y	46	7MG	C6-N1	-2.25	1.34	1.38
54	1y	46	7MG	C4-N9	-2.25	1.35	1.37
1	1A	2515	2MA	C2-N3	2.24	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1y	32	PSU	C4-N3	-2.24	1.34	1.38
32	2a	1498	UR3	C2-N1	2.23	1.41	1.38
54	1w	46	7MG	C8-N9	2.23	1.47	1.46
32	2a	1207	2MG	C6-N1	-2.23	1.34	1.37
55	1x	54	5MU	C2-N1	2.23	1.42	1.38
55	2x	54	5MU	C2-N1	2.22	1.42	1.38
1	1A	1937	5MU	C2-N1	2.22	1.42	1.38
32	2a	1404	5MC	C6-N1	-2.21	1.34	1.38
54	2w	8	4SU	C5-C4	-2.20	1.39	1.42
1	2A	1942	5MC	C6-N1	-2.19	1.34	1.38
1	2A	2503	2MA	C2-N3	2.18	1.35	1.31
1	1A	1937	5MU	C2-N3	-2.17	1.34	1.38
32	1a	967	5MC	C6-N1	-2.17	1.34	1.38
32	2a	967	5MC	C6-N1	-2.16	1.34	1.38
32	1a	527	7MG	C8-N9	2.16	1.47	1.46
1	1A	2617	PSU	C2-N1	-2.15	1.33	1.36
1	2A	2552	2MU	C4-N3	-2.15	1.34	1.38
1	1A	1984	5MC	C6-C5	2.14	1.38	1.34
32	2a	1400	5MC	C6-N1	-2.14	1.34	1.38
54	1y	54	5MU	C2-N3	-2.14	1.34	1.38
54	2y	46	7MG	C2-N3	2.13	1.38	1.33
54	2w	46	7MG	C5-C6	2.13	1.49	1.43
1	1A	2564	2MU	C5-C4	2.12	1.48	1.43
1	2A	1915	5MU	C6-N1	-2.12	1.34	1.38
1	1A	1939	PSU	C2-N3	-2.11	1.33	1.37
54	1w	37	MIA	C6-N1	2.10	1.35	1.32
1	2A	1939	5MU	C2-N3	-2.10	1.34	1.38
1	1A	1937	5MU	C6-N1	-2.10	1.34	1.38
54	2w	54	5MU	C2-N1	2.09	1.41	1.38
55	1x	54	5MU	C6-N1	-2.08	1.34	1.38
54	2y	55	PSU	C2-N1	-2.08	1.33	1.36
54	2w	37	MIA	C6-N1	2.07	1.35	1.32
1	1A	2617	PSU	C2-N3	-2.05	1.34	1.37
54	2w	46	7MG	C6-N1	-2.03	1.35	1.38
1	1A	1937	5MU	C4-C5	2.02	1.48	1.44
54	1y	54	5MU	C6-N1	-2.02	1.34	1.38
54	1y	8	4SU	C6-C5	2.02	1.39	1.35
55	2x	8	4SU	C6-C5	2.02	1.39	1.35
54	1y	32	PSU	C4-C5	2.01	1.49	1.44
32	2a	1407	5MC	C6-N1	-2.00	1.34	1.38
1	2A	2605	PSU	C2-N3	-2.00	1.34	1.37

All (325) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	2y	46	7MG	N9-C4-N3	9.81	140.14	125.47
54	1y	46	7MG	N9-C4-N3	8.86	138.72	125.47
54	2w	46	7MG	N9-C4-N3	8.78	138.60	125.47
32	2a	527	7MG	N9-C4-N3	8.63	138.38	125.47
54	1w	37	MIA	C12-C13-C14	-8.59	110.43	127.14
32	1a	527	7MG	N9-C4-N3	8.58	138.31	125.47
54	1w	46	7MG	N9-C4-N3	8.44	138.09	125.47
43	1l	92	0TD	CSB-SB-CB	-7.95	88.06	102.44
54	2w	8	4SU	C4-N3-C2	-7.17	120.38	127.34
1	2A	1917	PSU	N1-C2-N3	6.26	122.22	115.13
54	2w	55	PSU	N1-C2-N3	6.22	122.18	115.13
1	1A	1933	PSU	N1-C2-N3	6.20	122.16	115.13
54	1w	8	4SU	C4-N3-C2	-6.20	121.32	127.34
54	2y	8	4SU	C4-N3-C2	-6.16	121.36	127.34
54	2y	8	4SU	C5-C4-N3	6.14	120.38	114.69
54	1y	55	PSU	N1-C2-N3	6.11	122.05	115.13
1	1A	1939	PSU	N1-C2-N3	6.08	122.02	115.13
32	1a	1498	UR3	C4-N3-C2	-6.07	118.85	124.56
1	2A	1939	5MU	C4-N3-C2	-6.04	119.53	127.35
32	2a	1498	UR3	C4-N3-C2	-5.98	118.94	124.56
1	2A	2605	PSU	N1-C2-N3	5.94	121.86	115.13
55	2x	54	5MU	C4-N3-C2	-5.87	119.75	127.35
54	2w	8	4SU	C5-C4-N3	5.85	120.11	114.69
1	2A	1911	PSU	N1-C2-N3	5.76	121.66	115.13
1	1A	2564	2MU	N3-C2-N1	5.76	122.54	114.89
55	2x	55	PSU	N1-C2-N3	5.73	121.63	115.13
54	1w	55	PSU	N1-C2-N3	5.72	121.61	115.13
54	2w	32	PSU	N1-C2-N3	5.72	121.61	115.13
55	1x	55	PSU	N1-C2-N3	5.71	121.60	115.13
54	1w	39	PSU	N1-C2-N3	5.70	121.59	115.13
54	1w	32	PSU	N1-C2-N3	5.66	121.54	115.13
54	2y	46	7MG	C5-C4-N3	-5.66	117.35	128.13
54	2y	32	PSU	N1-C2-N3	5.62	121.50	115.13
54	1y	8	4SU	C4-N3-C2	-5.59	121.91	127.34
55	2x	54	5MU	N3-C2-N1	5.56	122.28	114.89
32	2a	516	PSU	N1-C2-N3	5.53	121.40	115.13
54	1y	39	PSU	N1-C2-N3	5.52	121.39	115.13
54	2y	39	PSU	N1-C2-N3	5.50	121.37	115.13
54	2w	46	7MG	N9-C8-N7	-5.50	95.51	103.38
54	1w	8	4SU	C5-C4-N3	5.50	119.79	114.69
1	1A	1937	5MU	C4-N3-C2	-5.48	120.25	127.35
54	1w	46	7MG	N9-C8-N7	-5.46	95.56	103.38
1	1A	1937	5MU	C5-C4-N3	5.46	119.97	115.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	527	7MG	N9-C8-N7	-5.42	95.63	103.38
32	1a	527	7MG	C5-C4-N3	-5.41	117.81	128.13
1	1A	1961	5MU	C4-N3-C2	-5.41	120.35	127.35
54	1y	32	PSU	N1-C2-N3	5.41	121.25	115.13
32	1a	516	PSU	N1-C2-N3	5.39	121.24	115.13
1	2A	1915	5MU	C4-N3-C2	-5.35	120.42	127.35
1	2A	1939	5MU	N3-C2-N1	5.32	121.95	114.89
54	2w	46	7MG	C5-C4-N3	-5.31	118.00	128.13
1	2A	1939	5MU	C5-C4-N3	5.25	119.79	115.31
1	2A	2552	2MU	N3-C2-N1	5.25	121.86	114.89
1	1A	2617	PSU	N1-C2-N3	5.24	121.07	115.13
32	2a	527	7MG	C5-C4-N3	-5.19	118.25	128.13
54	1y	46	7MG	N9-C8-N7	-5.18	95.97	103.38
1	1A	1961	5MU	C5-C4-N3	5.16	119.72	115.31
1	2A	1915	5MU	N3-C2-N1	5.12	121.69	114.89
1	1A	2564	2MU	C4-N3-C2	-5.08	119.88	126.58
54	1y	46	7MG	C5-C4-N3	-5.04	118.53	128.13
55	1x	54	5MU	N3-C2-N1	5.03	121.57	114.89
54	2w	39	PSU	N1-C2-N3	5.02	120.82	115.13
54	2y	55	PSU	N1-C2-N3	4.97	120.76	115.13
1	1A	1937	5MU	N3-C2-N1	4.96	121.47	114.89
1	1A	1961	5MU	O4-C4-C5	-4.94	119.17	124.90
32	1a	527	7MG	N9-C8-N7	-4.90	96.37	103.38
54	1y	54	5MU	N3-C2-N1	4.84	121.32	114.89
54	1y	54	5MU	C4-N3-C2	-4.84	121.08	127.35
1	1A	1937	5MU	O4-C4-C5	-4.77	119.37	124.90
1	1A	1961	5MU	N3-C2-N1	4.73	121.17	114.89
54	2y	46	7MG	C2-N3-C4	4.67	120.61	112.30
1	2A	1939	5MU	C5-C6-N1	-4.66	118.54	123.34
54	2y	46	7MG	N9-C8-N7	-4.63	96.75	103.38
54	2y	54	5MU	C5-C4-N3	4.60	119.24	115.31
54	2y	54	5MU	C4-N3-C2	-4.51	121.51	127.35
55	2x	54	5MU	C5-C4-N3	4.49	119.15	115.31
54	1w	46	7MG	C5-C4-N3	-4.48	119.60	128.13
1	2A	1915	5MU	C5-C4-N3	4.45	119.11	115.31
54	1w	37	MIA	C15-C14-C13	-4.40	109.93	122.65
54	1y	54	5MU	C5-C4-N3	4.40	119.07	115.31
55	1x	54	5MU	C4-N3-C2	-4.39	121.67	127.35
54	2w	46	7MG	C2-N3-C4	4.36	120.06	112.30
32	1a	527	7MG	C2-N3-C4	4.33	120.02	112.30
54	1w	54	5MU	N3-C2-N1	4.31	120.61	114.89
1	2A	1939	5MU	O4-C4-C5	-4.30	119.92	124.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	527	7MG	C2-N3-C4	4.27	119.91	112.30
54	1y	8	4SU	N3-C2-N1	4.26	120.54	114.89
54	2w	37	MIA	C2-N3-C4	4.24	121.17	115.32
1	2A	2552	2MU	C4-N3-C2	-4.24	120.99	126.58
1	1A	2564	2MU	O2-C2-N1	-4.23	117.16	122.79
54	1w	54	5MU	C4-N3-C2	-4.22	121.89	127.35
54	2y	8	4SU	C5-C4-S4	-4.22	119.03	124.47
54	2w	55	PSU	C4-N3-C2	-4.20	120.29	126.34
54	2w	8	4SU	N3-C2-N1	4.19	120.46	114.89
54	2w	54	5MU	C4-N3-C2	-4.19	121.92	127.35
54	1y	46	7MG	C2-N3-C4	4.18	119.75	112.30
54	1w	37	MIA	C5-C6-N1	-4.15	117.36	120.81
54	1w	37	MIA	C11-S10-C2	-4.15	99.17	102.27
54	1y	8	4SU	C5-C4-N3	4.12	118.51	114.69
1	1A	1961	5MU	C5-C6-N1	-4.11	119.11	123.34
1	2A	2605	PSU	C4-N3-C2	-4.09	120.44	126.34
55	1x	55	PSU	C4-N3-C2	-4.08	120.46	126.34
1	1A	1933	PSU	C4-N3-C2	-4.08	120.46	126.34
54	2y	54	5MU	N3-C2-N1	4.05	120.27	114.89
55	2x	55	PSU	C4-N3-C2	-4.03	120.53	126.34
54	2w	54	5MU	C5-C4-N3	4.02	118.74	115.31
54	2y	54	5MU	O4-C4-C5	-3.99	120.28	124.90
1	1A	1984	5MC	C5-C6-N1	-3.97	119.25	123.34
55	2x	54	5MU	O4-C4-C5	-3.96	120.31	124.90
54	2w	54	5MU	O4-C4-C5	-3.91	120.36	124.90
32	1a	516	PSU	O2-C2-N1	-3.90	118.49	122.79
54	1w	55	PSU	C4-N3-C2	-3.90	120.72	126.34
1	2A	1915	5MU	C5-C6-N1	-3.90	119.33	123.34
54	2w	37	MIA	C5-C6-N1	-3.89	117.58	120.81
54	2w	54	5MU	N3-C2-N1	3.89	120.05	114.89
54	1w	54	5MU	C5-C4-N3	3.88	118.62	115.31
55	2x	54	5MU	C5-C6-N1	-3.86	119.37	123.34
54	1w	37	MIA	C16-C14-C13	-3.84	111.55	122.65
32	2a	516	PSU	C4-N3-C2	-3.81	120.85	126.34
54	1w	32	PSU	C4-N3-C2	-3.80	120.86	126.34
32	1a	1400	5MC	C5-C6-N1	-3.79	119.44	123.34
1	2A	1917	PSU	O2-C2-N1	-3.78	118.63	122.79
32	1a	967	5MC	C5-C6-N1	-3.77	119.45	123.34
54	1y	54	5MU	C5-C6-N1	-3.77	119.46	123.34
54	2y	37	MIA	N3-C2-N1	-3.75	122.82	128.68
1	1A	1933	PSU	O2-C2-N1	-3.74	118.67	122.79
54	1y	55	PSU	O2-C2-N1	-3.74	118.68	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	1939	PSU	O2-C2-N1	-3.73	118.68	122.79
54	1w	37	MIA	C2-N3-C4	3.72	120.45	115.32
54	1w	8	4SU	C5-C4-S4	-3.70	119.70	124.47
1	2A	1917	PSU	C4-N3-C2	-3.69	121.02	126.34
54	2w	8	4SU	C5-C4-S4	-3.68	119.73	124.47
54	2y	55	PSU	C4-N3-C2	-3.68	121.04	126.34
54	1y	55	PSU	C4-N3-C2	-3.67	121.05	126.34
55	2x	54	5MU	O2-C2-N1	-3.67	117.91	122.79
54	1w	46	7MG	C2-N3-C4	3.67	118.83	112.30
32	1a	516	PSU	C4-N3-C2	-3.66	121.06	126.34
1	1A	1939	PSU	C4-N3-C2	-3.64	121.09	126.34
54	2y	32	PSU	C4-N3-C2	-3.64	121.10	126.34
54	1y	37	MIA	N3-C2-N1	-3.63	123.00	128.68
1	2A	1911	PSU	C4-N3-C2	-3.63	121.11	126.34
54	2y	55	PSU	O2-C2-N1	-3.63	118.80	122.79
54	1w	8	4SU	N3-C2-N1	3.60	119.67	114.89
1	2A	1962	5MC	C5-C6-N1	-3.60	119.63	123.34
32	2a	967	5MC	C5-C6-N1	-3.59	119.65	123.34
55	1x	8	4SU	C6-C5-C4	-3.58	116.85	119.95
55	2x	8	4SU	C5-C4-N3	3.58	118.01	114.69
54	2w	32	PSU	C4-N3-C2	-3.57	121.19	126.34
54	2y	39	PSU	C4-N3-C2	-3.54	121.24	126.34
32	1a	1518	MA6	C4-C5-N7	-3.53	105.72	109.40
54	2y	8	4SU	N3-C2-N1	3.53	119.57	114.89
55	1x	8	4SU	C5-C4-N3	3.51	117.94	114.69
32	1a	1519	MA6	N1-C6-N6	3.50	120.74	117.06
32	2a	1519	MA6	C4-C5-N7	-3.49	105.76	109.40
54	1w	39	PSU	C4-N3-C2	-3.49	121.31	126.34
1	2A	2605	PSU	O2-C2-N1	-3.46	118.98	122.79
1	2A	1915	5MU	O4-C4-C5	-3.46	120.89	124.90
1	1A	2617	PSU	C4-N3-C2	-3.46	121.35	126.34
54	1w	39	PSU	O2-C2-N1	-3.43	119.01	122.79
54	2y	54	5MU	C1'-N1-C2	3.43	123.78	117.57
1	2A	1939	5MU	O2-C2-N1	-3.42	118.24	122.79
1	1A	1937	5MU	C5-C6-N1	-3.42	119.82	123.34
54	1y	54	5MU	O4-C4-C5	-3.39	120.97	124.90
55	2x	32	5MC	C5-C6-N1	-3.39	119.86	123.34
32	1a	1518	MA6	N3-C2-N1	-3.38	123.39	128.68
55	1x	54	5MU	O4-C4-C5	-3.38	120.98	124.90
54	2w	32	PSU	O2-C2-N1	-3.37	119.08	122.79
55	1x	32	5MC	C5-C6-N1	-3.36	119.88	123.34
32	2a	1404	5MC	C5-C6-N1	-3.35	119.89	123.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2A	2552	2MU	O2-C2-N1	-3.33	118.37	122.79
1	1A	2617	PSU	O2-C2-N1	-3.32	119.13	122.79
54	1y	32	PSU	C4-N3-C2	-3.32	121.56	126.34
32	1a	1404	5MC	C5-C6-N1	-3.32	119.93	123.34
32	2a	1518	MA6	C9-N6-C6	-3.31	109.48	119.51
54	1w	32	PSU	O2-C2-N1	-3.30	119.16	122.79
32	2a	1407	5MC	C5-C6-N1	-3.29	119.95	123.34
54	2y	54	5MU	C1'-N1-C6	-3.26	115.69	121.12
32	2a	1518	MA6	C4-C5-N7	-3.24	106.03	109.40
1	1A	1964	5MC	C5-C6-N1	-3.23	120.01	123.34
54	1y	39	PSU	C4-N3-C2	-3.23	121.69	126.34
32	2a	1519	MA6	C9-N6-C6	-3.22	109.78	119.51
43	1l	92	0TD	OD2-CG-CB	3.21	120.09	113.15
54	1w	55	PSU	O2-C2-N1	-3.21	119.26	122.79
54	2w	55	PSU	O2-C2-N1	-3.20	119.27	122.79
1	2A	1942	5MC	C5-C6-N1	-3.19	120.06	123.34
55	1x	54	5MU	C5-C4-N3	3.18	118.03	115.31
32	1a	1518	MA6	C9-N6-C6	-3.18	109.90	119.51
54	2y	39	PSU	O2-C2-N1	-3.14	119.33	122.79
54	1y	32	PSU	O2-C2-N1	-3.14	119.34	122.79
54	1w	54	5MU	C5-C6-N1	-3.13	120.12	123.34
54	1w	46	7MG	C5-C4-N9	-3.13	102.28	106.35
32	1a	1519	MA6	N3-C2-N1	-3.13	123.79	128.68
32	1a	1407	5MC	C5-C6-N1	-3.11	120.13	123.34
32	2a	1404	5MC	C5-C4-N3	-3.11	118.32	121.67
32	2a	1518	MA6	N3-C2-N1	-3.07	123.88	128.68
55	2x	8	4SU	C1'-N1-C2	3.07	123.12	117.57
32	1a	1519	MA6	C4-C5-N7	-3.05	106.22	109.40
55	1x	8	4SU	O2-C2-N1	3.01	126.79	122.79
1	1A	2564	2MU	O4-C4-C5	-3.01	119.87	125.16
43	2l	92	0TD	OD2-CG-CB	3.01	119.65	113.15
55	1x	55	PSU	O2-C2-N1	-2.98	119.50	122.79
1	2A	1911	PSU	O2-C2-N1	-2.98	119.51	122.79
54	2y	46	7MG	C5-C4-N9	-2.96	102.50	106.35
1	1A	2564	2MU	C5-C4-N3	2.96	119.27	114.84
54	2y	32	PSU	O2-C2-N1	-2.94	119.55	122.79
54	2w	39	PSU	C4-N3-C2	-2.93	122.12	126.34
54	1w	54	5MU	O4-C4-C5	-2.91	121.53	124.90
32	2a	1407	5MC	C5-C4-N3	-2.91	118.53	121.67
1	2A	2503	2MA	C5-C6-N1	2.90	119.02	114.02
54	2w	54	5MU	C5-C6-N1	-2.88	120.37	123.34
54	1y	37	MIA	C4-C5-N7	-2.87	106.41	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	2y	54	5MU	C5-C6-N1	-2.86	120.39	123.34
55	1x	54	5MU	C5-C6-N1	-2.86	120.39	123.34
1	2A	2552	2MU	O4-C4-C5	-2.86	120.13	125.16
32	2a	527	7MG	C5-C6-N1	2.84	116.00	110.99
54	2w	46	7MG	C5-C6-N1	2.84	116.00	110.99
32	1a	1519	MA6	C9-N6-C6	-2.83	110.93	119.51
32	1a	1400	5MC	C5-C4-N3	-2.83	118.62	121.67
32	1a	1407	5MC	C5-C4-N3	-2.82	118.63	121.67
1	1A	1964	5MC	C5-C4-N3	-2.80	118.65	121.67
54	2w	8	4SU	C1'-N1-C2	2.78	122.61	117.57
54	2w	37	MIA	C2-N1-C6	2.78	122.17	117.19
54	2w	37	MIA	C4-C5-N7	-2.78	106.50	109.40
54	1y	46	7MG	C5-C4-N9	-2.78	102.74	106.35
54	2w	37	MIA	C12-N6-C6	-2.76	120.49	122.87
55	1x	32	5MC	C5-C4-N3	-2.76	118.69	121.67
54	1w	37	MIA	C2-N1-C6	2.73	122.08	117.19
32	2a	1519	MA6	N3-C2-N1	-2.73	124.41	128.68
32	2a	1400	5MC	C5-C6-N1	-2.70	120.56	123.34
54	1w	54	5MU	C5M-C5-C4	2.63	121.66	118.77
54	2y	54	5MU	O2-C2-N3	-2.62	116.61	121.50
1	2A	1942	5MC	C5-C4-N3	-2.62	118.84	121.67
32	2a	1402	4OC	C6-C5-C4	2.61	120.15	116.96
55	2x	32	5MC	C5-C4-N3	-2.60	118.87	121.67
32	1a	527	7MG	C5-C6-N1	2.59	115.56	110.99
32	2a	516	PSU	O2-C2-N1	-2.58	119.95	122.79
54	1y	8	4SU	C5-C4-S4	-2.57	121.15	124.47
54	2w	37	MIA	C11-S10-C2	-2.57	100.35	102.27
32	1a	1207	2MG	C8-N7-C5	2.57	107.89	102.99
54	1w	37	MIA	C4-C5-N7	-2.56	106.73	109.40
1	2A	2503	2MA	C8-N7-C5	2.56	107.87	102.99
32	2a	1407	5MC	O2-C2-N3	-2.55	118.19	122.33
32	2a	1402	4OC	O2-C2-N3	-2.54	118.20	122.33
32	2a	967	5MC	C5-C4-N3	-2.54	118.93	121.67
32	2a	1207	2MG	C8-N7-C5	2.54	107.82	102.99
55	2x	55	PSU	O2-C2-N1	-2.53	120.00	122.79
32	2a	1518	MA6	C10-N6-C9	-2.52	108.01	116.12
1	1A	1984	5MC	CM5-C5-C6	-2.51	119.50	122.85
32	1a	1404	5MC	C5-C4-N3	-2.51	118.97	121.67
1	2A	2251	OMG	C8-N7-C5	2.50	107.75	102.99
1	1A	2263	OMG	C8-N7-C5	2.49	107.74	102.99
54	1w	37	MIA	C12-N6-C6	-2.49	118.85	122.55
32	1a	516	PSU	C6-C5-C4	-2.49	116.46	118.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	1400	5MC	C5-C4-N3	-2.44	119.04	121.67
32	2a	1519	MA6	N1-C6-N6	2.44	119.62	117.06
55	2x	32	5MC	O2-C2-N3	-2.44	118.37	122.33
32	1a	1207	2MG	CM2-N2-C2	-2.43	118.50	123.86
55	2x	8	4SU	O2-C2-N1	2.42	126.00	122.79
1	1A	2515	2MA	C5-C6-N1	2.39	118.14	114.02
1	1A	2515	2MA	C8-N7-C5	2.38	107.53	102.99
55	2x	8	4SU	O2-C2-N3	-2.38	117.06	121.50
32	2a	967	5MC	O2-C2-N3	-2.35	118.51	122.33
1	1A	2617	PSU	C6-C5-C4	-2.34	116.56	118.20
32	1a	1402	4OC	C6-C5-C4	2.34	119.82	116.96
1	2A	2251	OMG	C5-C6-N1	2.33	118.08	113.95
43	2l	92	0TD	OD1-CG-CB	-2.32	117.58	122.44
1	2A	2552	2MU	C5-C4-N3	2.32	118.31	114.84
54	2y	54	5MU	C5M-C5-C4	2.31	121.31	118.77
32	1a	966	M2G	C8-N7-C5	2.31	107.39	102.99
54	2w	37	MIA	N3-C2-N1	-2.30	122.75	126.98
32	1a	966	M2G	C5-C6-N1	2.30	118.01	113.95
32	2a	527	7MG	C5-C4-N9	-2.30	103.36	106.35
54	2w	46	7MG	C5-C4-N9	-2.29	103.37	106.35
32	2a	1498	UR3	C1'-N1-C2	2.29	120.85	116.99
1	1A	1961	5MU	O2-C2-N1	-2.27	119.77	122.79
32	1a	1498	UR3	C1'-N1-C2	2.26	120.80	116.99
54	1y	46	7MG	C5-C6-N1	2.25	114.96	110.99
32	1a	1518	MA6	C10-N6-C6	-2.25	112.71	119.51
54	2y	37	MIA	C4-C5-N7	-2.24	107.06	109.40
32	1a	1518	MA6	C10-N6-C9	-2.23	108.94	116.12
54	2y	8	4SU	C1'-N1-C2	2.22	121.59	117.57
55	1x	54	5MU	O2-C2-N1	-2.21	119.85	122.79
1	1A	2263	OMG	C5-C6-N1	2.21	117.85	113.95
32	2a	966	M2G	C5-C6-N1	2.20	117.84	113.95
54	2w	37	MIA	N6-C6-N1	2.20	121.24	118.50
54	1y	54	5MU	O2-C2-N3	-2.19	117.42	121.50
32	2a	527	7MG	CM7-N7-C5	2.19	132.06	126.40
1	1A	1937	5MU	O2-C2-N1	-2.19	119.88	122.79
1	1A	1964	5MC	O2-C2-N3	-2.18	118.78	122.33
32	2a	516	PSU	O4'-C1'-C2'	2.18	108.21	105.14
54	2w	55	PSU	C5-C6-N1	-2.17	118.85	122.11
54	2w	54	5MU	C5M-C5-C4	2.17	121.16	118.77
43	1l	92	0TD	OD1-CG-CB	-2.16	117.91	122.44
55	2x	55	PSU	C5-C6-N1	-2.16	118.86	122.11
54	1y	39	PSU	O2-C2-N1	-2.16	120.42	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	2y	46	7MG	C5-C6-N1	2.15	114.78	110.99
55	1x	55	PSU	C5-C6-N1	-2.14	118.90	122.11
54	2w	39	PSU	C6-C5-C4	-2.13	116.71	118.20
54	1y	55	PSU	O4'-C1'-C2'	2.12	108.14	105.14
1	2A	1915	5MU	C5M-C5-C6	-2.12	120.02	122.85
55	1x	8	4SU	C1'-N1-C2	2.11	121.39	117.57
54	1w	37	MIA	N3-C2-N1	-2.11	123.11	126.98
32	2a	966	M2G	C8-N7-C5	2.10	107.00	102.99
54	1w	46	7MG	CM7-N7-C5	2.10	131.81	126.40
54	1y	8	4SU	C1'-N1-C2	2.10	121.36	117.57
1	1A	2564	2MU	C2'-C1'-N1	-2.09	110.16	114.22
32	1a	1400	5MC	CM5-C5-C6	-2.09	120.05	122.85
55	1x	54	5MU	C5M-C5-C4	2.09	121.07	118.77
54	2y	37	MIA	C2-N1-C6	2.09	122.33	118.75
32	1a	527	7MG	CM7-N7-C5	2.09	131.79	126.40
54	2w	46	7MG	O6-C6-C5	-2.09	122.42	127.54
54	2y	55	PSU	O4'-C1'-C2'	2.09	108.09	105.14
54	2w	39	PSU	O2-C2-N1	-2.08	120.50	122.79
32	1a	967	5MC	C5-C4-N3	-2.08	119.43	121.67
54	2y	46	7MG	CM7-N7-C5	2.07	131.75	126.40
54	2y	55	PSU	C6-C5-C4	-2.07	116.75	118.20
1	2A	2251	OMG	CM2-O2'-C2'	-2.07	109.09	114.52
55	1x	8	4SU	O2-C2-N3	-2.07	117.65	121.50
55	1x	32	5MC	O2-C2-N3	-2.07	118.97	122.33
54	2y	32	PSU	O4'-C1'-C2'	2.06	108.05	105.14
1	2A	1915	5MU	C5M-C5-C4	2.06	121.03	118.77
32	1a	1404	5MC	CM5-C5-C6	-2.05	120.11	122.85
1	2A	1962	5MC	C5-C4-N3	-2.05	119.46	121.67
32	1a	516	PSU	O4'-C1'-C2'	2.03	108.01	105.14
32	2a	1518	MA6	N1-C6-N6	2.01	119.17	117.06

There are no chirality outliers.

All (72) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1A	2263	OMG	C1'-C2'-O2'-CM2
32	1a	527	7MG	C3'-C4'-C5'-O5'
32	1a	1518	MA6	C5-C6-N6-C10
32	1a	1519	MA6	O4'-C4'-C5'-O5'
43	1l	92	0TD	O-C-CA-CB
54	1w	37	MIA	C12-C13-C14-C16
54	1y	46	7MG	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
54	1y	54	5MU	O4'-C4'-C5'-O5'
32	2a	1518	MA6	C5-C6-N6-C10
32	2a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
32	2a	1519	MA6	C5-C6-N6-C10
54	2w	46	7MG	O4'-C4'-C5'-O5'
54	2w	46	7MG	C3'-C4'-C5'-O5'
54	2y	37	MIA	C3'-C4'-C5'-O5'
54	2y	55	PSU	C2'-C1'-C5-C6
54	2y	55	PSU	O4'-C1'-C5-C6
32	1a	1519	MA6	C3'-C4'-C5'-O5'
54	1y	54	5MU	C3'-C4'-C5'-O5'
32	2a	967	5MC	O4'-C4'-C5'-O5'
54	1y	8	4SU	C3'-C4'-C5'-O5'
54	1y	8	4SU	O4'-C4'-C5'-O5'
1	2A	1917	PSU	O4'-C4'-C5'-O5'
32	2a	967	5MC	C3'-C4'-C5'-O5'
54	2y	46	7MG	O4'-C1'-N9-C4
32	1a	527	7MG	O4'-C4'-C5'-O5'
55	1x	55	PSU	O4'-C4'-C5'-O5'
54	2y	37	MIA	O4'-C4'-C5'-O5'
54	2w	37	MIA	N1-C6-N6-C12
32	1a	1519	MA6	C5-C6-N6-C10
32	2a	1518	MA6	C5-C6-N6-C9
32	2a	1402	4OC	O4'-C4'-C5'-O5'
32	2a	527	7MG	C3'-C4'-C5'-O5'
32	1a	1400	5MC	O4'-C4'-C5'-O5'
1	2A	2552	2MU	O4'-C4'-C5'-O5'
54	2y	32	PSU	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C4'-C5'-O5'-P
43	2l	92	0TD	CG-CB-SB-CSB
54	1w	46	7MG	C2'-C1'-N9-C8
54	2w	46	7MG	C2'-C1'-N9-C8
54	2y	46	7MG	C2'-C1'-N9-C8
1	1A	1942	4OC	C3'-C2'-O2'-CM2
54	2y	46	7MG	O4'-C1'-N9-C8
32	2a	527	7MG	C4'-C5'-O5'-P
54	2y	37	MIA	C4'-C5'-O5'-P
1	2A	1917	PSU	C3'-C4'-C5'-O5'
32	1a	527	7MG	C4'-C5'-O5'-P
54	1w	46	7MG	C4'-C5'-O5'-P
54	1y	8	4SU	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
54	1y	46	7MG	C2'-C1'-N9-C8
54	2y	54	5MU	C2'-C1'-N1-C2
54	2y	54	5MU	C2'-C1'-N1-C6
54	1y	55	PSU	O4'-C1'-C5-C4
32	1a	967	5MC	O4'-C4'-C5'-O5'
1	2A	2503	2MA	O4'-C4'-C5'-O5'
32	1a	1400	5MC	C3'-C4'-C5'-O5'
55	1x	55	PSU	C3'-C4'-C5'-O5'
32	2a	1207	2MG	O4'-C4'-C5'-O5'
32	2a	1402	4OC	C3'-C4'-C5'-O5'
54	1w	46	7MG	O4'-C1'-N9-C8
1	1A	2515	2MA	C4'-C5'-O5'-P
32	2a	527	7MG	O4'-C4'-C5'-O5'
43	1l	92	0TD	CG-CB-SB-CSB
55	2x	8	4SU	C2'-C1'-N1-C2
1	1A	2515	2MA	O4'-C4'-C5'-O5'
32	2a	1404	5MC	C3'-C4'-C5'-O5'
54	2y	32	PSU	C3'-C4'-C5'-O5'
54	2y	55	PSU	O4'-C4'-C5'-O5'
32	2a	1402	4OC	C2'-C1'-N1-C2
54	2y	8	4SU	C2'-C1'-N1-C2
54	1y	54	5MU	C4'-C5'-O5'-P
54	2w	46	7MG	O4'-C1'-N9-C8

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 2280 ligands modelled in this entry, 2271 are monoatomic - leaving 9 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	$\#\|Z\|>2$
57	KAN	2A	3568	56	35,35,35	1.55	6 (17%)	46,52,52	1.43	5 (10%)
57	KAN	1A	3934	-	35,35,35	1.50	5 (14%)	46,52,52	1.60	9 (19%)
59	SF4	2d	501	35	0,12,12	-	-	-		
57	KAN	1A	3933	-	35,35,35	1.70	6 (17%)	46,52,52	1.29	7 (15%)
57	KAN	1A	3935	56	35,35,35	1.68	7 (20%)	46,52,52	1.74	12 (26%)
57	KAN	2A	3569	56	35,35,35	1.57	6 (17%)	46,52,52	1.92	13 (28%)
57	KAN	2a	1828	-	35,35,35	1.65	6 (17%)	46,52,52	1.36	6 (13%)
57	KAN	1a	1955	-	35,35,35	1.64	7 (20%)	46,52,52	1.11	5 (10%)
59	SF4	1d	303	35	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	KAN	2A	3568	56	-	4/12/72/72	0/3/3/3
57	KAN	1A	3934	-	-	4/12/72/72	0/3/3/3
59	SF4	2d	501	35	-	-	0/6/5/5
57	KAN	1A	3933	-	-	4/12/72/72	0/3/3/3
57	KAN	1A	3935	56	-	2/12/72/72	0/3/3/3
57	KAN	2A	3569	56	-	2/12/72/72	0/3/3/3
57	KAN	2a	1828	-	-	1/12/72/72	0/3/3/3
57	KAN	1a	1955	-	-	3/12/72/72	0/3/3/3
59	SF4	1d	303	35	-	-	0/6/5/5

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	1A	3933	KAN	C14-C15	-5.68	1.46	1.53
57	2a	1828	KAN	C14-C15	-5.67	1.46	1.53
57	1A	3935	KAN	C14-C15	-5.25	1.46	1.53
57	1a	1955	KAN	C14-C15	-5.24	1.47	1.53
57	2A	3568	KAN	C14-C15	-5.12	1.47	1.53
57	1A	3934	KAN	C14-C15	-4.16	1.48	1.53
57	1A	3933	KAN	C16-C15	-4.07	1.48	1.53
57	1A	3935	KAN	C16-C15	-4.01	1.48	1.53
57	2A	3569	KAN	C14-C15	-3.98	1.48	1.53
57	2A	3569	KAN	O12-C13	3.89	1.51	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	1A	3934	KAN	C15-N4	3.62	1.52	1.47
57	1a	1955	KAN	C16-C15	-3.61	1.49	1.53
57	2A	3569	KAN	C16-C15	-3.52	1.49	1.53
57	2A	3569	KAN	C15-N4	3.41	1.52	1.47
57	1a	1955	KAN	O12-C13	3.21	1.50	1.41
57	2A	3568	KAN	C15-N4	3.15	1.52	1.47
57	2a	1828	KAN	O12-C13	3.14	1.49	1.41
57	1A	3935	KAN	C15-N4	3.12	1.52	1.47
57	2A	3568	KAN	O12-C13	3.09	1.49	1.41
57	2A	3568	KAN	C16-C15	-3.08	1.49	1.53
57	1a	1955	KAN	C15-N4	3.08	1.52	1.47
57	1A	3934	KAN	C16-C15	-3.07	1.49	1.53
57	1A	3933	KAN	C15-N4	2.97	1.51	1.47
57	1A	3935	KAN	O12-C13	2.97	1.49	1.41
57	1A	3934	KAN	O12-C13	2.90	1.49	1.41
57	2a	1828	KAN	C16-C15	-2.90	1.49	1.53
57	2a	1828	KAN	C15-N4	2.79	1.51	1.47
57	1A	3933	KAN	O12-C13	2.77	1.48	1.41
57	1A	3935	KAN	O11-C13	-2.48	1.34	1.41
57	2a	1828	KAN	O5-C1	2.48	1.48	1.41
57	2A	3569	KAN	O5-C1	2.47	1.48	1.41
57	2a	1828	KAN	O5-C5	2.47	1.50	1.44
57	1A	3933	KAN	O5-C5	2.44	1.50	1.44
57	1A	3933	KAN	O5-C1	2.37	1.47	1.41
57	1A	3934	KAN	O5-C5	2.30	1.49	1.44
57	2A	3569	KAN	O5-C5	2.27	1.49	1.44
57	1A	3935	KAN	C6-C5	-2.23	1.49	1.52
57	1A	3935	KAN	O9-C1	-2.22	1.35	1.41
57	1a	1955	KAN	O5-C1	2.19	1.47	1.41
57	1a	1955	KAN	C6-C5	-2.15	1.49	1.52
57	1a	1955	KAN	O5-C5	2.13	1.49	1.44
57	2A	3568	KAN	O5-C1	2.10	1.47	1.41
57	2A	3568	KAN	C6-C5	-2.10	1.49	1.52

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	2A	3568	KAN	O12-C17-C16	5.00	118.78	109.69
57	2a	1828	KAN	O12-C17-C16	4.65	118.14	109.69
57	2A	3568	KAN	C13-O11-C8	-4.57	106.66	117.96
57	2A	3569	KAN	C4-C3-C2	4.49	118.66	110.82
57	1A	3933	KAN	C10-C9-C8	4.40	118.08	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	1A	3934	KAN	C13-O12-C17	-3.89	106.06	113.69
57	2A	3569	KAN	C3-C4-C5	3.73	116.89	110.24
57	1A	3934	KAN	O11-C8-C9	3.58	116.80	107.28
57	1A	3935	KAN	C13-C14-C15	-3.47	105.74	110.40
57	1A	3935	KAN	C13-O11-C8	-3.41	109.53	117.96
57	2A	3569	KAN	O5-C1-C2	3.39	117.52	110.35
57	1A	3935	KAN	O9-C1-O5	-3.38	101.24	110.67
57	1A	3935	KAN	C1-O9-C10	-3.35	109.68	117.96
57	2A	3569	KAN	O5-C5-C6	3.33	112.20	106.01
57	2A	3569	KAN	C1-C2-C3	3.31	116.90	110.00
57	2A	3569	KAN	C11-C12-C7	3.27	117.90	111.18
57	2A	3569	KAN	O12-C17-C16	3.27	115.63	109.69
57	1A	3933	KAN	O12-C17-C16	3.26	115.62	109.69
57	2a	1828	KAN	C13-C14-C15	-3.26	106.01	110.40
57	1A	3934	KAN	O9-C10-C9	3.22	115.86	107.28
57	2A	3569	KAN	C1-O9-C10	-3.19	110.06	117.96
57	1A	3935	KAN	O12-C17-C16	3.18	115.46	109.69
57	1A	3935	KAN	C10-C9-C8	3.14	115.48	108.96
57	1A	3934	KAN	C3-C4-C5	3.08	115.74	110.24
57	1A	3935	KAN	C4-C3-C2	3.07	116.18	110.82
57	2a	1828	KAN	C13-O11-C8	-2.93	110.72	117.96
57	2A	3569	KAN	C13-C14-C15	2.91	114.31	110.40
57	2A	3569	KAN	O11-C8-C7	-2.88	102.31	109.18
57	1A	3934	KAN	C10-C9-C8	-2.88	102.99	108.96
57	1A	3934	KAN	C6-C5-C4	-2.84	107.51	113.10
57	1a	1955	KAN	C13-O11-C8	-2.82	110.98	117.96
57	1A	3935	KAN	O5-C1-C2	2.80	116.28	110.35
57	1a	1955	KAN	C18-C17-C16	-2.67	106.76	113.00
57	1A	3935	KAN	C18-C17-C16	-2.66	106.77	113.00
57	2A	3569	KAN	C12-C11-C10	2.63	116.17	109.53
57	1A	3935	KAN	C1-C2-C3	2.61	115.44	110.00
57	1A	3934	KAN	C4-C3-C2	2.60	115.36	110.82
57	2a	1828	KAN	C6-C5-C4	-2.58	108.03	113.10
57	2A	3569	KAN	O12-C13-C14	2.47	115.58	110.35
57	1A	3935	KAN	C1-O5-C5	-2.45	108.88	113.69
57	2a	1828	KAN	O5-C5-C6	2.41	110.49	106.01
57	1A	3934	KAN	O5-C5-C4	2.33	113.92	109.69
57	1A	3933	KAN	C13-O11-C8	-2.33	112.21	117.96
57	2A	3569	KAN	C10-C9-C8	2.32	113.78	108.96
57	2a	1828	KAN	O9-C1-C2	-2.31	102.10	108.10
57	2A	3568	KAN	C1-O9-C10	-2.22	112.46	117.96
57	1A	3934	KAN	O9-C10-C11	2.14	114.30	109.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	1A	3933	KAN	C18-C17-C16	-2.14	107.98	113.00
57	2A	3568	KAN	O14-C16-C15	-2.12	106.42	110.22
57	2A	3568	KAN	C1-O5-C5	-2.10	109.56	113.69
57	1A	3935	KAN	C16-C15-C14	-2.09	106.52	111.06
57	1a	1955	KAN	C10-C9-C8	2.09	113.30	108.96
57	1a	1955	KAN	O12-C17-C16	2.08	113.47	109.69
57	1A	3933	KAN	O5-C5-C6	2.03	109.78	106.01
57	1a	1955	KAN	O9-C10-C11	-2.02	104.37	109.18
57	1A	3933	KAN	C12-C11-C10	2.01	114.61	109.53
57	1A	3933	KAN	C6-C5-C4	-2.00	109.16	113.10

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	2A	3568	KAN	C11-C10-O9-C1
57	1A	3934	KAN	C9-C8-O11-C13
57	1A	3935	KAN	O12-C17-C18-O15
57	1A	3933	KAN	O12-C17-C18-O15
57	1a	1955	KAN	O12-C17-C18-O15
57	1A	3935	KAN	C16-C17-C18-O15
57	2A	3568	KAN	O12-C17-C18-O15
57	1A	3934	KAN	C9-C10-O9-C1
57	1a	1955	KAN	C16-C17-C18-O15
57	1A	3933	KAN	O5-C1-O9-C10
57	2a	1828	KAN	O12-C17-C18-O15
57	1A	3933	KAN	C2-C1-O9-C10
57	2A	3569	KAN	O12-C17-C18-O15
57	1A	3934	KAN	O12-C17-C18-O15
57	2A	3568	KAN	C9-C10-O9-C1
57	2A	3568	KAN	C16-C17-C18-O15
57	1A	3933	KAN	C16-C17-C18-O15
57	1a	1955	KAN	C9-C10-O9-C1
57	2A	3569	KAN	O12-C13-O11-C8
57	1A	3934	KAN	C4-C5-C6-N1

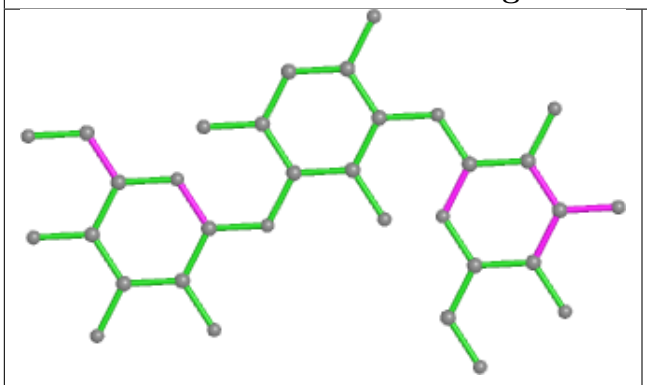
There are no ring outliers.

No monomer is involved in short contacts.

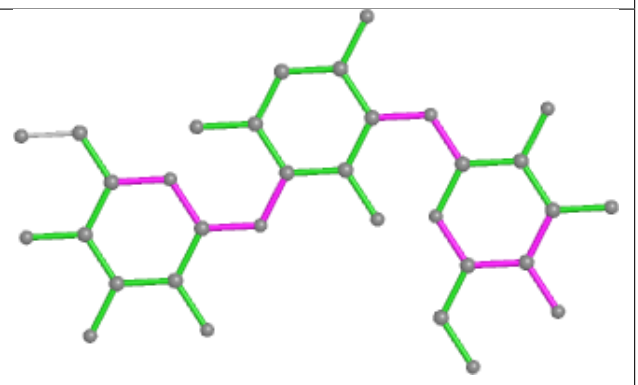
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

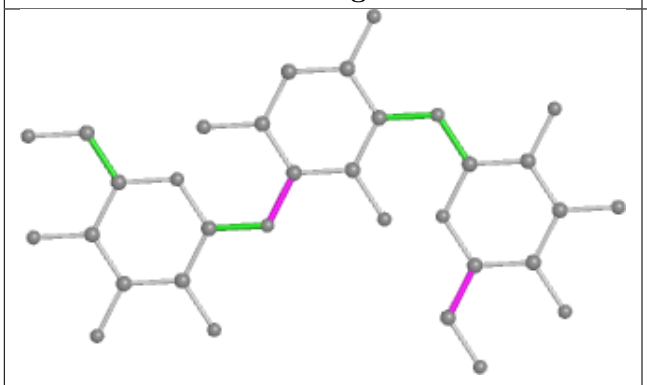
Ligand KAN 2A 3568



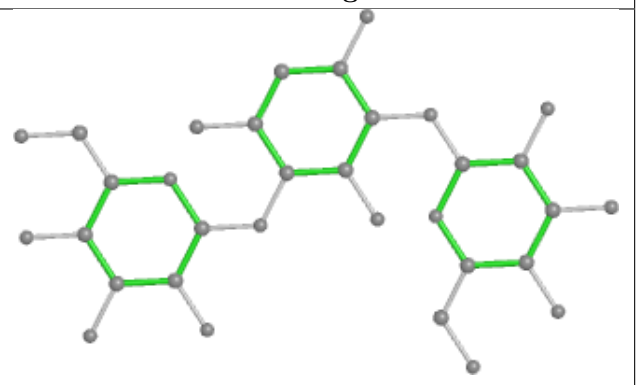
Bond lengths



Bond angles

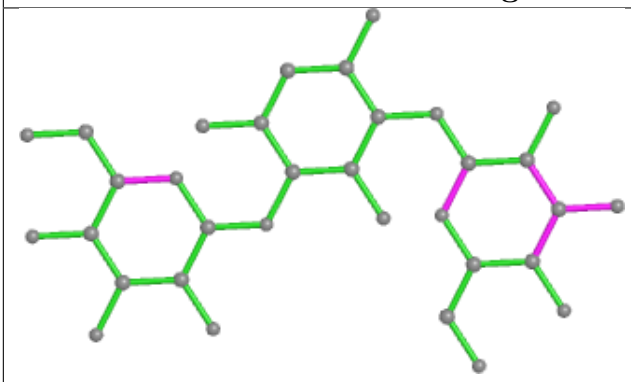


Torsions

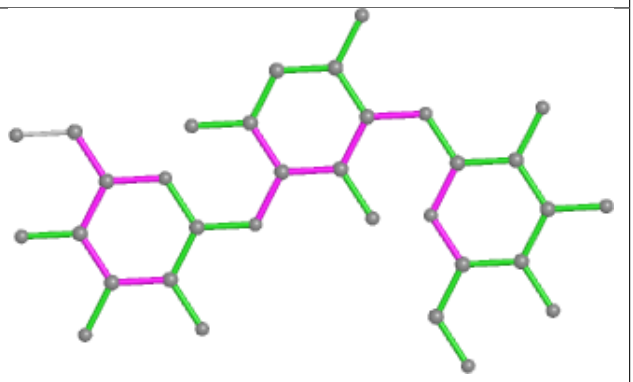


Rings

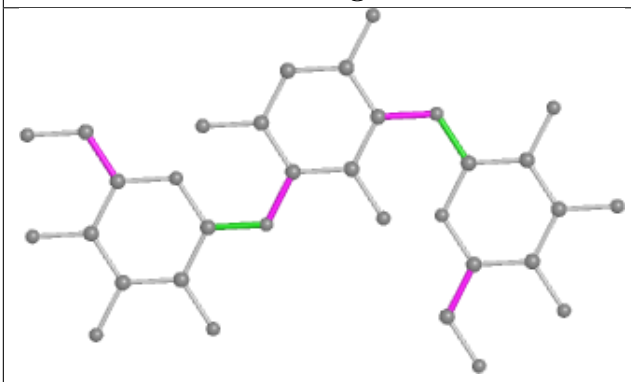
Ligand KAN 1A 3934



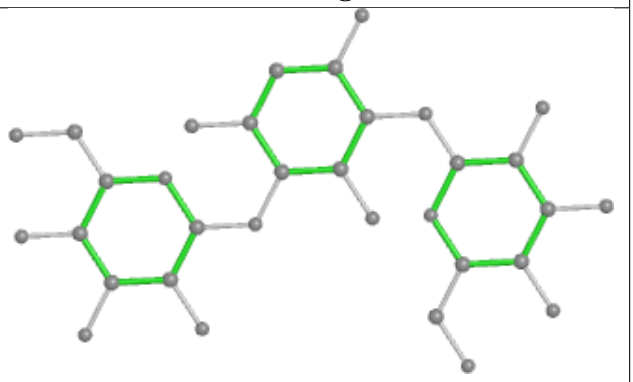
Bond lengths



Bond angles

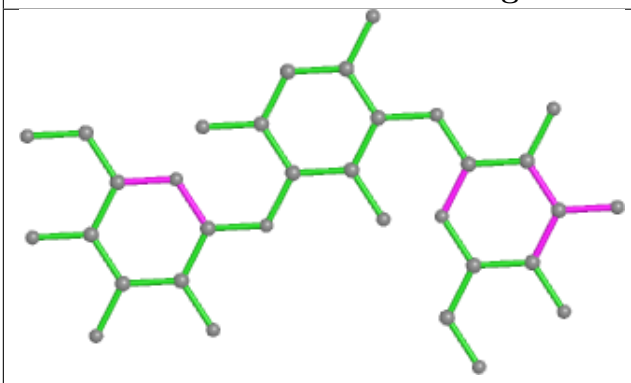


Torsions

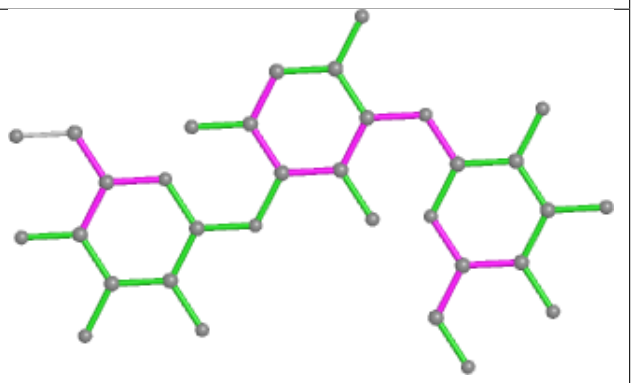


Rings

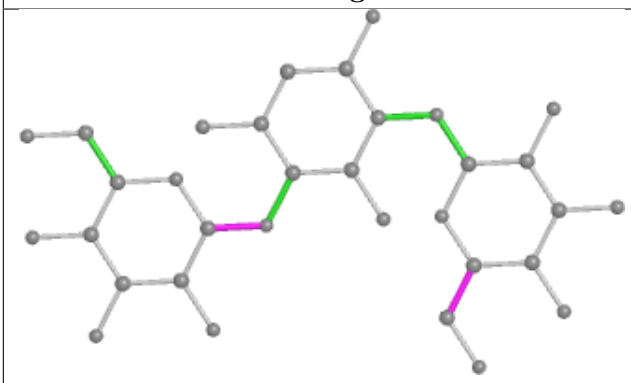
Ligand KAN 1A 3933



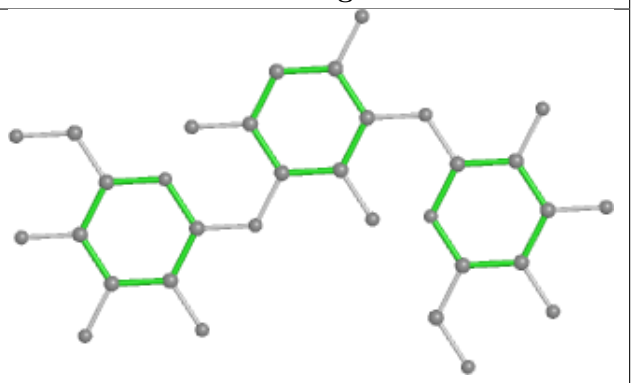
Bond lengths



Bond angles

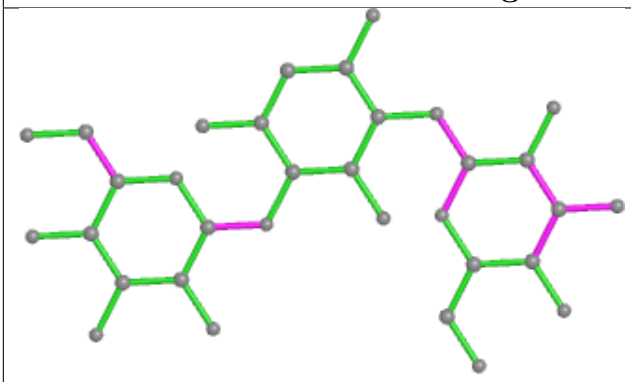


Torsions

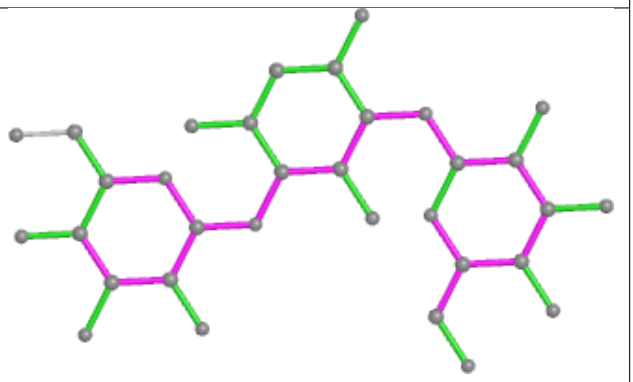


Rings

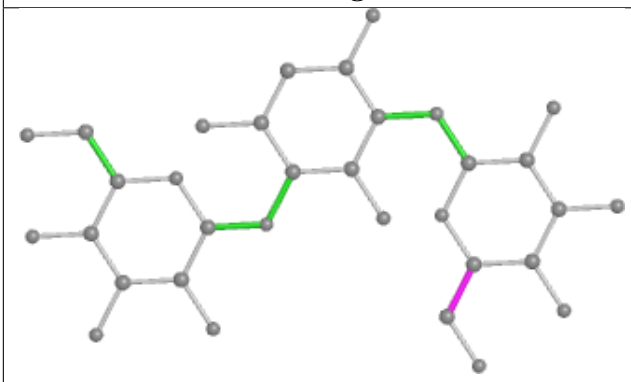
Ligand KAN 1A 3935



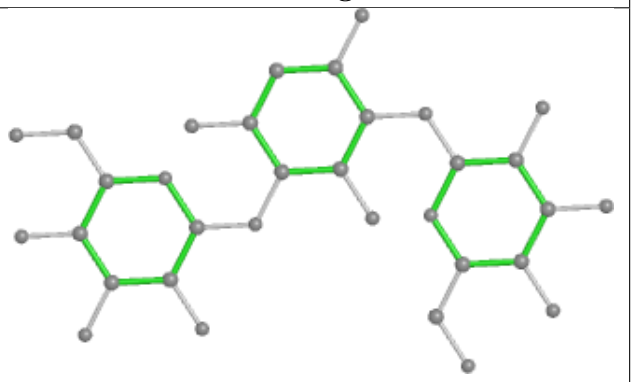
Bond lengths



Bond angles

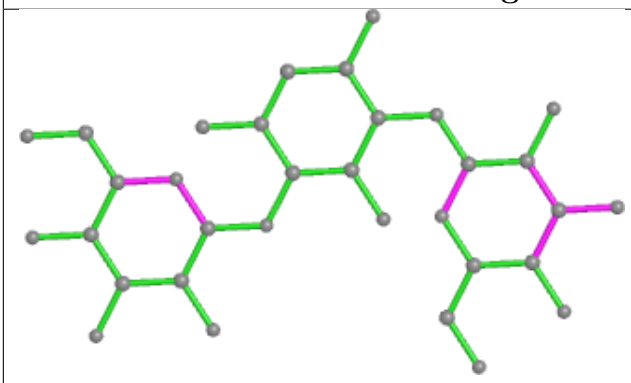


Torsions

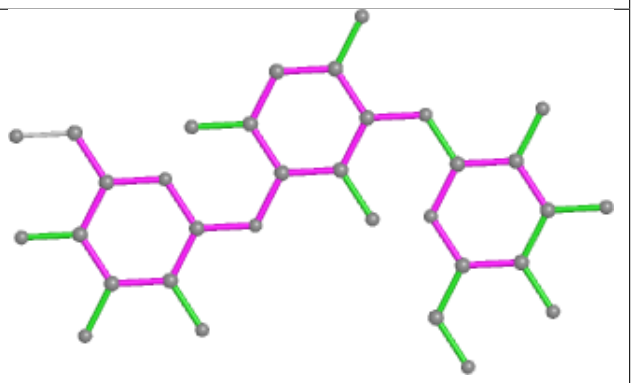


Rings

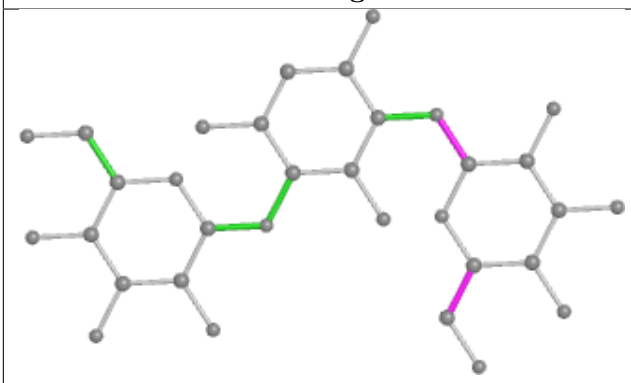
Ligand KAN 2A 3569



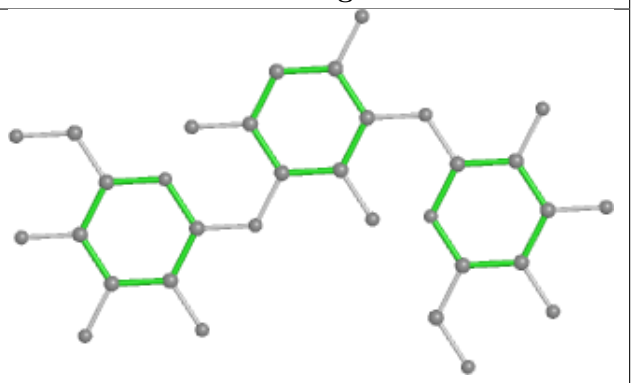
Bond lengths



Bond angles

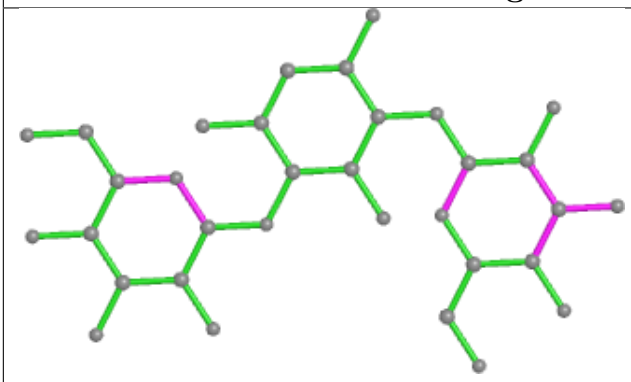


Torsions

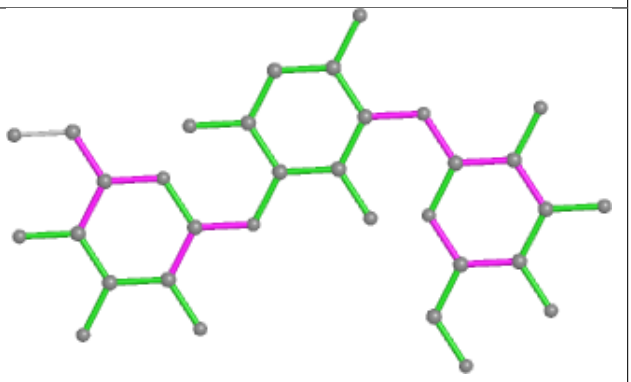


Rings

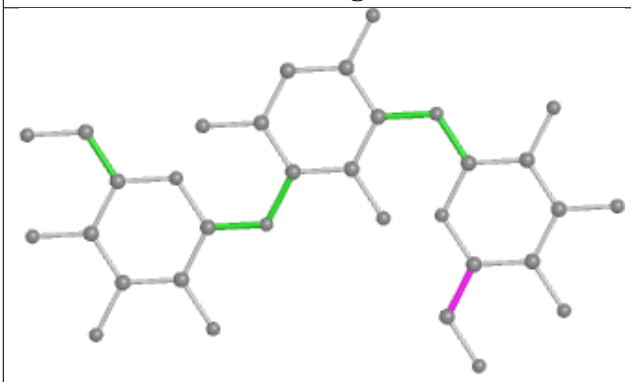
Ligand KAN 2a 1828



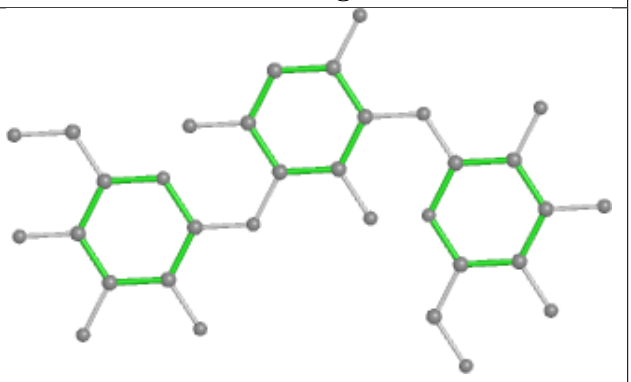
Bond lengths



Bond angles

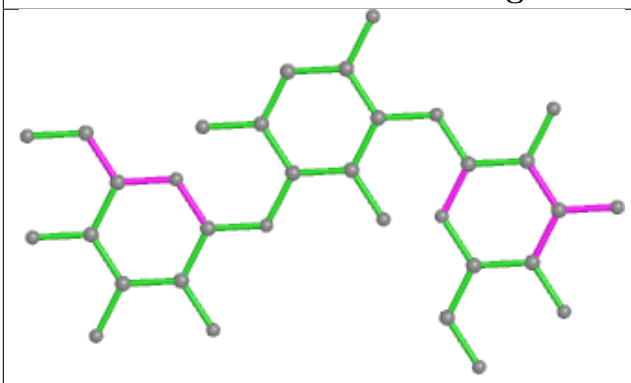


Torsions

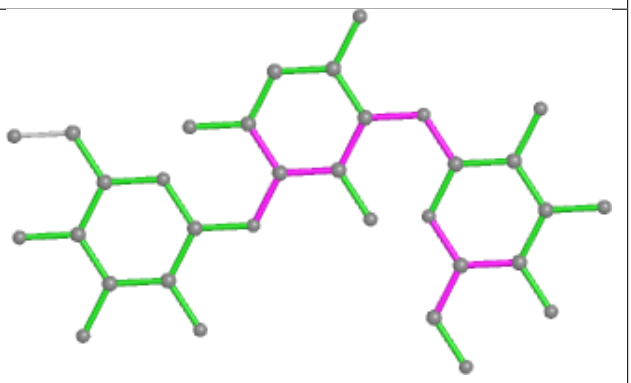


Rings

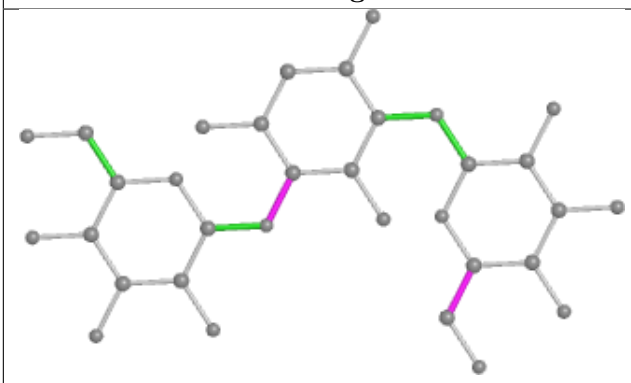
Ligand KAN 1a 1955



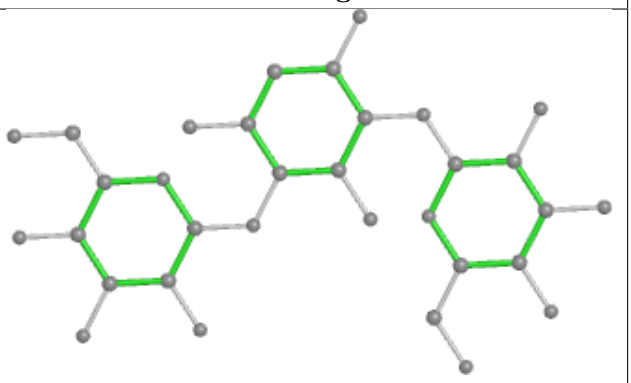
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} 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%)	0.04	28 (0%) 82 82	23, 43, 106, 122	0
1	2A	2789/2915 (95%)	0.01	26 (0%) 84 84	38, 65, 105, 122	0
2	1B	120/121 (99%)	-0.26	0 100 100	37, 56, 75, 100	0
2	2B	120/121 (99%)	-0.15	0 100 100	69, 87, 98, 111	0
3	1D	275/276 (99%)	0.38	4 (1%) 73 73	25, 44, 60, 83	0
3	2D	275/276 (99%)	0.35	4 (1%) 73 73	36, 56, 69, 83	0
4	1E	204/206 (99%)	0.16	0 100 100	27, 46, 67, 86	0
4	2E	204/206 (99%)	0.34	5 (2%) 57 55	39, 68, 80, 91	0
5	1F	203/210 (96%)	0.12	0 100 100	24, 49, 75, 96	0
5	2F	203/210 (96%)	0.46	10 (4%) 29 26	43, 75, 91, 103	0
6	1G	181/182 (99%)	0.50	12 (6%) 18 14	46, 64, 81, 96	0
6	2G	181/182 (99%)	1.36	50 (27%) 0 0	74, 88, 97, 104	0
7	1H	174/180 (96%)	-0.03	2 (1%) 80 80	45, 62, 75, 81	0
7	2H	174/180 (96%)	1.64	59 (33%) 0 0	77, 91, 102, 106	0
8	1I	146/148 (98%)	0.34	6 (4%) 37 32	51, 82, 93, 97	0
8	2I	146/148 (98%)	0.54	13 (8%) 9 7	65, 86, 96, 101	0
9	1N	140/140 (100%)	0.28	0 100 100	34, 46, 69, 79	0
9	2N	140/140 (100%)	0.83	17 (12%) 4 3	55, 73, 88, 93	0
10	1O	122/122 (100%)	0.34	1 (0%) 86 86	33, 46, 64, 70	0
10	2O	122/122 (100%)	0.33	1 (0%) 86 86	52, 64, 78, 86	0
11	1P	149/150 (99%)	0.16	1 (0%) 87 87	23, 51, 76, 86	0
11	2P	149/150 (99%)	0.85	20 (13%) 3 2	46, 76, 92, 100	0
12	1Q	141/141 (100%)	0.39	4 (2%) 53 49	34, 47, 60, 86	0
12	2Q	141/141 (100%)	1.22	31 (21%) 0 0	58, 76, 88, 98	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	1R	118/118 (100%)	0.45	0 100 100	29, 40, 53, 64	0
13	2R	118/118 (100%)	0.20	2 (1%) 70 69	47, 59, 70, 77	0
14	1S	110/112 (98%)	0.09	2 (1%) 68 67	42, 56, 68, 76	0
14	2S	110/112 (98%)	1.11	18 (16%) 1 1	70, 81, 90, 94	0
15	1T	131/146 (89%)	0.07	0 100 100	39, 50, 76, 95	0
15	2T	131/146 (89%)	0.36	8 (6%) 21 17	56, 68, 88, 96	0
16	1U	116/118 (98%)	0.20	2 (1%) 70 69	27, 37, 54, 71	0
16	2U	116/118 (98%)	0.32	3 (2%) 56 52	49, 70, 82, 89	0
17	1V	101/101 (100%)	0.06	1 (0%) 82 82	28, 46, 62, 79	0
17	2V	101/101 (100%)	0.51	6 (5%) 22 18	50, 79, 90, 93	0
18	1W	112/113 (99%)	0.37	2 (1%) 68 67	26, 38, 59, 92	0
18	2W	112/113 (99%)	0.49	1 (0%) 84 84	45, 56, 75, 96	0
19	1X	95/96 (98%)	0.17	0 100 100	30, 44, 66, 87	0
19	2X	95/96 (98%)	0.99	14 (14%) 2 1	48, 67, 81, 90	0
20	1Y	107/110 (97%)	0.11	1 (0%) 84 84	47, 57, 80, 89	0
20	2Y	107/110 (97%)	1.20	27 (25%) 0 0	69, 81, 94, 95	0
21	1Z	154/206 (74%)	0.55	13 (8%) 11 8	50, 67, 93, 100	0
21	2Z	160/206 (77%)	1.04	31 (19%) 1 0	77, 92, 105, 111	0
22	10	83/85 (97%)	0.69	7 (8%) 11 8	33, 44, 72, 89	0
22	20	83/85 (97%)	1.30	22 (26%) 0 0	52, 72, 86, 95	0
23	11	97/98 (98%)	0.32	2 (2%) 63 61	28, 45, 76, 80	0
23	21	97/98 (98%)	0.82	9 (9%) 8 6	46, 62, 84, 97	0
24	12	70/72 (97%)	0.03	1 (1%) 75 75	42, 54, 65, 94	0
24	22	70/72 (97%)	0.41	1 (1%) 75 75	61, 78, 87, 89	0
25	13	59/60 (98%)	-0.06	1 (1%) 70 69	30, 42, 66, 84	0
25	23	59/60 (98%)	1.43	14 (23%) 0 0	65, 74, 90, 102	0
26	14	69/71 (97%)	0.81	11 (15%) 1 1	57, 81, 99, 107	0
26	24	69/71 (97%)	0.92	16 (23%) 0 0	87, 95, 106, 110	0
27	15	59/60 (98%)	0.18	1 (1%) 70 69	26, 39, 57, 70	0
27	25	59/60 (98%)	0.07	1 (1%) 70 69	46, 60, 75, 79	0
28	16	53/54 (98%)	-0.08	0 100 100	34, 46, 61, 68	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	26	53/54 (98%)	0.78	5 (9%) 8 6	57, 65, 77, 82	0
29	17	48/49 (97%)	0.17	1 (2%) 63 61	30, 34, 65, 72	0
29	27	48/49 (97%)	0.52	4 (8%) 11 8	37, 46, 70, 82	0
30	18	64/65 (98%)	0.11	0 100 100	31, 39, 48, 65	0
30	28	64/65 (98%)	1.22	11 (17%) 1 1	48, 63, 70, 76	0
31	19	37/37 (100%)	0.39	0 100 100	39, 46, 66, 70	0
31	29	37/37 (100%)	2.01	17 (45%) 0 0	67, 78, 90, 92	0
32	1a	1488/1521 (97%)	-0.12	10 (0%) 87 87	42, 71, 104, 121	0
32	2a	1491/1521 (98%)	-0.10	16 (1%) 80 80	55, 85, 106, 122	0
33	1b	231/256 (90%)	0.51	18 (7%) 13 10	72, 89, 104, 110	0
33	2b	231/256 (90%)	1.44	68 (29%) 0 0	84, 97, 104, 110	0
34	1c	206/239 (86%)	0.67	21 (10%) 6 5	60, 76, 89, 94	0
34	2c	206/239 (86%)	1.10	52 (25%) 0 0	84, 94, 100, 107	0
35	1d	208/209 (99%)	0.47	9 (4%) 35 31	58, 74, 88, 98	0
35	2d	208/209 (99%)	0.97	36 (17%) 1 1	67, 80, 93, 101	0
36	1e	148/162 (91%)	0.39	4 (2%) 54 50	58, 69, 81, 94	0
36	2e	148/162 (91%)	0.62	14 (9%) 8 6	78, 86, 94, 102	0
37	1f	100/101 (99%)	0.14	2 (2%) 65 63	57, 72, 83, 86	0
37	2f	100/101 (99%)	0.27	1 (1%) 82 82	64, 77, 86, 96	0
38	1g	155/156 (99%)	0.48	14 (9%) 9 7	63, 75, 91, 102	0
38	2g	155/156 (99%)	0.77	19 (12%) 4 3	76, 87, 98, 113	0
39	1h	137/138 (99%)	0.63	16 (11%) 4 3	62, 74, 82, 89	0
39	2h	137/138 (99%)	0.79	17 (12%) 4 3	74, 86, 93, 97	0
40	1i	127/128 (99%)	0.82	20 (15%) 2 1	59, 81, 91, 94	0
40	2i	127/128 (99%)	2.10	61 (48%) 0 0	79, 94, 101, 105	0
41	1j	97/105 (92%)	0.83	12 (12%) 4 3	58, 83, 96, 101	0
41	2j	96/105 (91%)	1.36	26 (27%) 0 0	84, 95, 104, 110	0
42	1k	114/129 (88%)	0.48	4 (3%) 44 38	52, 72, 83, 87	0
42	2k	114/129 (88%)	0.97	18 (15%) 2 1	63, 81, 90, 93	0
43	1l	121/132 (91%)	0.15	1 (0%) 86 86	47, 56, 73, 82	0
43	2l	121/132 (91%)	0.74	11 (9%) 9 6	60, 73, 84, 87	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	1m	123/126 (97%)	0.61	8 (6%) 18 14	60, 72, 85, 98	0
44	2m	122/126 (96%)	1.37	29 (23%) 0 0	78, 92, 98, 105	0
45	1n	60/61 (98%)	0.73	6 (10%) 7 5	61, 70, 77, 82	0
45	2n	60/61 (98%)	2.32	30 (50%) 0 0	83, 92, 98, 99	0
46	1o	88/89 (98%)	0.16	1 (1%) 80 80	57, 69, 83, 91	0
46	2o	88/89 (98%)	0.58	4 (4%) 33 29	64, 81, 89, 95	0
47	1p	82/88 (93%)	0.79	10 (12%) 4 3	62, 74, 85, 96	0
47	2p	82/88 (93%)	0.98	17 (20%) 1 0	64, 76, 86, 92	0
48	1q	99/105 (94%)	0.02	2 (2%) 65 63	57, 73, 84, 89	0
48	2q	99/105 (94%)	0.95	15 (15%) 2 1	68, 80, 89, 95	0
49	1r	68/88 (77%)	0.44	2 (2%) 51 47	61, 72, 85, 88	0
49	2r	68/88 (77%)	0.50	7 (10%) 6 5	64, 81, 90, 96	0
50	1s	83/93 (89%)	0.14	3 (3%) 42 37	62, 75, 84, 94	0
50	2s	83/93 (89%)	0.60	8 (9%) 8 6	87, 94, 102, 107	0
51	1t	96/106 (90%)	0.81	11 (11%) 4 3	64, 77, 88, 95	0
51	2t	96/106 (90%)	0.95	14 (14%) 2 1	65, 77, 91, 94	0
52	1u	23/27 (85%)	0.78	5 (21%) 0 0	64, 72, 77, 80	0
52	2u	23/27 (85%)	2.56	13 (56%) 0 0	80, 89, 93, 94	0
53	1v	13/24 (54%)	0.50	1 (7%) 13 10	50, 62, 88, 105	0
53	2v	13/24 (54%)	1.46	4 (30%) 0 0	75, 95, 115, 118	0
54	1w	67/76 (88%)	0.57	7 (10%) 6 5	60, 98, 112, 115	0
54	1y	67/76 (88%)	0.22	4 (5%) 21 18	44, 104, 112, 121	0
54	2w	65/76 (85%)	0.97	12 (18%) 1 0	85, 108, 116, 120	0
54	2y	66/76 (86%)	0.63	6 (9%) 9 6	62, 113, 118, 119	0
55	1x	72/77 (93%)	-0.05	0 100 100	45, 72, 93, 99	0
55	2x	72/77 (93%)	0.05	0 100 100	61, 86, 100, 106	0
All	All	20875/21748 (95%)	0.34	1238 (5%) 22 18	23, 70, 100, 122	0

All (1238) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
44	2m	123	ALA	14.8
44	1m	124	PRO	12.7

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Mol	Chain	Res	Type	RSRZ
44	2m	124	PRO	12.0
38	2g	82	GLY	11.4
21	2Z	144	LEU	11.1
44	1m	123	ALA	9.2
22	10	8	GLY	8.5
22	10	7	LEU	8.4
19	2X	92	LEU	8.1
45	2n	39	LEU	8.1
33	2b	165	VAL	7.8
45	2n	34	TYR	7.8
35	2d	167	GLY	7.7
45	2n	25	VAL	7.5
33	2b	37	ASN	7.5
41	2j	47	PHE	7.2
21	2Z	170	THR	6.9
45	2n	2	ALA	6.8
22	10	6	GLY	6.8
23	11	2	SER	6.7
31	29	37	GLY	6.7
31	29	12	ASP	6.6
25	23	60	GLU	6.5
38	2g	81	GLY	6.5
23	21	2	SER	6.4
40	2i	27	THR	6.4
38	1g	80	VAL	6.3
41	2j	55	LYS	6.3
44	2m	102	ARG	6.2
53	2v	24	A	6.2
44	2m	122	LYS	6.2
38	1g	84	ASN	6.1
1	2A	883	G	6.0
54	2w	71	G	5.9
6	2G	2	PRO	5.9
33	2b	118	LEU	5.8
7	2H	89	ILE	5.8
45	2n	38	GLY	5.8
40	2i	127	LYS	5.7
32	2a	1030(B)	C	5.7
7	2H	159	GLU	5.7
1	1A	942	A	5.6
34	2c	198	VAL	5.6
26	14	54	GLY	5.6

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Mol	Chain	Res	Type	RSRZ
40	2i	101	PHE	5.5
33	2b	232	PRO	5.5
27	15	60	VAL	5.4
33	2b	187	LEU	5.4
31	29	17	ILE	5.3
52	2u	17	THR	5.3
34	2c	146	ALA	5.3
20	2Y	5	MET	5.3
35	2d	165	MET	5.2
33	2b	233	SER	5.2
50	2s	80	TYR	5.2
12	2Q	109	VAL	5.1
29	27	48	LYS	5.1
33	2b	121	LEU	5.1
32	2a	1257	U	5.1
38	1g	82	GLY	5.0
42	2k	35	PRO	5.0
40	2i	7	THR	5.0
1	2A	896	A	5.0
7	2H	105	LEU	5.0
38	2g	80	VAL	5.0
1	1A	1555	C	5.0
21	2Z	149	SER	4.9
12	2Q	66	ILE	4.9
12	2Q	104	PHE	4.9
33	1b	77	ALA	4.9
41	2j	62	HIS	4.9
7	2H	103	LEU	4.9
1	2A	888	C	4.9
7	2H	49	VAL	4.9
40	2i	19	LEU	4.9
38	2g	156	TRP	4.9
35	2d	160	GLN	4.9
40	2i	125	TYR	4.9
44	2m	5	ALA	4.8
34	2c	204	LEU	4.8
19	2X	95	LEU	4.8
21	2Z	121	HIS	4.8
38	1g	79	ARG	4.8
6	2G	3	LEU	4.8
5	2F	131	GLY	4.7
6	2G	139	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
52	2u	13	ILE	4.7
20	2Y	55	TYR	4.7
6	2G	29	TRP	4.7
38	2g	7	ALA	4.7
44	2m	121	LYS	4.7
7	2H	169	VAL	4.7
41	2j	48	THR	4.7
31	29	15	LYS	4.7
42	2k	25	TYR	4.7
49	2r	87	ARG	4.7
20	2Y	1	MET	4.7
38	1g	85	TYR	4.7
12	2Q	113	GLN	4.6
36	2e	22	GLY	4.6
33	1b	33	TYR	4.6
12	2Q	103	MET	4.6
7	2H	166	GLY	4.6
34	2c	182	ILE	4.6
36	2e	13	ILE	4.6
50	2s	84	GLY	4.6
1	1A	932	C	4.6
40	1i	19	LEU	4.6
33	2b	48	MET	4.6
7	2H	45	VAL	4.6
45	2n	61	TRP	4.6
45	2n	36	PHE	4.6
54	2w	72	C	4.5
32	2a	1030(A)	G	4.5
6	2G	157	ILE	4.5
31	29	16	VAL	4.5
26	14	49	PHE	4.5
40	2i	17	VAL	4.5
34	2c	158	GLY	4.5
41	2j	96	ILE	4.5
52	2u	16	GLY	4.5
54	2y	34	G	4.5
33	2b	31	TYR	4.5
22	20	75	LEU	4.4
34	1c	193	TYR	4.4
21	2Z	147	GLY	4.4
40	2i	90	PRO	4.4
29	27	47	ARG	4.4

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Mol	Chain	Res	Type	RSRZ
6	2G	90	LEU	4.4
7	2H	94	TYR	4.4
1	2A	882	G	4.4
44	2m	119	GLY	4.4
33	2b	236	TYR	4.4
7	2H	13	LYS	4.4
21	2Z	155	LEU	4.3
33	2b	197	VAL	4.3
41	2j	63	PHE	4.3
42	2k	89	ALA	4.3
43	2l	69	TYR	4.3
52	2u	11	GLY	4.3
7	2H	115	VAL	4.3
21	2Z	145	GLU	4.3
34	2c	6	HIS	4.3
30	28	16	ILE	4.3
34	2c	14	ILE	4.3
7	2H	171	LEU	4.2
40	2i	81	ILE	4.2
14	2S	58	LEU	4.2
54	2w	76	A	4.2
41	2j	59	SER	4.2
33	2b	227	GLY	4.2
9	2N	8	GLN	4.2
40	2i	36	TYR	4.2
22	20	76	GLY	4.2
21	1Z	149	SER	4.2
41	1j	93	GLY	4.2
17	2V	94	LEU	4.1
36	2e	10	MET	4.1
51	2t	9	ASN	4.1
1	2A	229	A	4.1
43	2l	64	TYR	4.1
33	2b	211	ILE	4.1
9	2N	45	ASN	4.1
21	2Z	152	ALA	4.1
26	14	45	GLY	4.1
34	2c	160	ALA	4.1
32	1a	1030(B)	C	4.1
7	2H	48	GLY	4.1
12	2Q	106	VAL	4.1
8	2I	12	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
48	2q	74	LEU	4.1
44	2m	120	LYS	4.1
45	2n	35	ARG	4.1
35	2d	20	TYR	4.1
9	2N	140	VAL	4.1
6	2G	133	LEU	4.0
12	2Q	2	LEU	4.0
34	2c	142	MET	4.0
38	1g	83	ALA	4.0
1	2A	1509	C	4.0
33	2b	214	ILE	4.0
43	2l	26	ALA	4.0
6	2G	28	VAL	4.0
41	2j	98	ILE	4.0
14	2S	57	LYS	4.0
33	1b	232	PRO	4.0
40	2i	14	VAL	4.0
51	1t	55	ILE	4.0
6	1G	139	LEU	4.0
20	1Y	1	MET	4.0
1	1A	935	C	4.0
21	2Z	173	ALA	4.0
45	2n	11	LYS	3.9
6	2G	102	PHE	3.9
44	2m	4	ILE	3.9
33	2b	40	HIS	3.9
5	2F	196	LEU	3.9
8	2I	3	VAL	3.9
54	1w	71	G	3.9
22	20	68	GLU	3.9
34	2c	155	GLY	3.9
45	2n	37	PHE	3.9
7	2H	71	LEU	3.9
9	2N	44	PRO	3.9
45	2n	23	ARG	3.9
1	2A	884	C	3.9
34	2c	4	LYS	3.8
26	24	40	HIS	3.8
32	1a	204	U	3.8
35	2d	168	ARG	3.8
20	2Y	61	ILE	3.8
44	2m	6	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
20	2Y	35	TYR	3.8
20	2Y	58	GLY	3.8
41	2j	46	ARG	3.8
7	2H	113	VAL	3.8
34	2c	202	ILE	3.8
8	2I	85	GLU	3.8
40	2i	65	VAL	3.8
38	2g	154	TYR	3.8
44	2m	90	LEU	3.8
12	2Q	32	TYR	3.8
43	2l	32	PHE	3.8
54	1y	20	U	3.8
7	2H	168	PRO	3.8
40	2i	28	VAL	3.8
8	2I	86	THR	3.8
19	2X	18	TYR	3.8
29	17	48	LYS	3.8
18	1W	112	GLY	3.8
50	2s	82	GLY	3.8
20	2Y	45	VAL	3.8
40	2i	114	TYR	3.7
40	1i	47	LEU	3.7
20	2Y	46	LYS	3.7
34	2c	147	LYS	3.7
20	2Y	50	ARG	3.7
33	2b	92	TYR	3.7
49	1r	25	THR	3.7
52	2u	14	TRP	3.7
54	1w	70	G	3.7
49	2r	46	GLU	3.7
34	2c	207	VAL	3.7
22	20	7	LEU	3.7
39	2h	112	LEU	3.7
53	2v	14	A	3.7
41	1j	72	VAL	3.7
7	2H	129	THR	3.7
8	2I	19	VAL	3.7
19	2X	89	ILE	3.7
28	26	11	LEU	3.6
30	28	61	LEU	3.6
45	2n	57	ARG	3.6
40	2i	61	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
33	2b	122	PHE	3.6
54	2w	70	G	3.6
11	2P	123	LEU	3.6
28	26	5	VAL	3.6
40	2i	115	GLY	3.6
52	2u	2	GLY	3.6
49	2r	85	LEU	3.6
12	2Q	6	ARG	3.6
51	1t	83	ARG	3.6
14	2S	32	LEU	3.6
6	2G	137	GLU	3.6
25	23	6	VAL	3.6
40	2i	26	VAL	3.6
41	2j	68	HIS	3.6
17	2V	72	VAL	3.6
29	27	46	VAL	3.6
38	1g	81	GLY	3.6
9	2N	1	MET	3.6
6	2G	182	LYS	3.6
33	1b	233	SER	3.6
7	2H	102	ALA	3.6
1	2A	885	C	3.5
3	1D	276	LYS	3.5
32	1a	1030(C)	G	3.5
40	2i	88	TYR	3.5
26	24	49	PHE	3.5
40	2i	92	TYR	3.5
45	2n	55	GLY	3.5
12	2Q	37	LEU	3.5
51	2t	24	LEU	3.5
11	2P	95	VAL	3.5
23	21	62	VAL	3.5
35	2d	107	ARG	3.5
41	2j	65	LEU	3.5
14	2S	20	ARG	3.5
52	2u	10	ARG	3.5
52	2u	23	PRO	3.5
22	20	8	GLY	3.5
21	2Z	150	LEU	3.5
31	29	25	VAL	3.5
35	2d	158	ILE	3.5
48	2q	11	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
42	2k	16	SER	3.5
36	2e	90	VAL	3.5
33	2b	228	GLY	3.5
34	2c	33	LEU	3.5
35	2d	108	LEU	3.5
39	1h	59	LEU	3.5
32	1a	1257	U	3.5
45	1n	2	ALA	3.5
51	2t	13	LEU	3.5
11	2P	15	ARG	3.5
38	2g	4	ARG	3.5
34	2c	159	GLY	3.4
35	2d	166	LYS	3.4
6	2G	34	LEU	3.4
6	2G	89	GLY	3.4
7	2H	148	ILE	3.4
34	2c	60	ALA	3.4
34	2c	138	VAL	3.4
47	2p	33	ILE	3.4
33	2b	152	PHE	3.4
35	2d	49	ARG	3.4
34	2c	201	TYR	3.4
25	23	35	ARG	3.4
40	2i	110	GLU	3.4
7	2H	88	LEU	3.4
40	2i	49	PRO	3.4
44	1m	120	LYS	3.4
39	2h	95	VAL	3.4
46	2o	87	ILE	3.4
26	24	32	TYR	3.4
41	2j	11	PHE	3.4
35	2d	70	ILE	3.4
6	2G	136	ARG	3.4
34	2c	167	TRP	3.4
17	1V	101	GLY	3.4
1	2A	2146	C	3.4
35	2d	164	ALA	3.4
5	2F	146	ALA	3.4
21	2Z	139	VAL	3.4
12	2Q	63	LYS	3.4
30	28	21	LYS	3.4
34	1c	72	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
44	2m	13	LYS	3.4
38	2g	85	TYR	3.4
53	1v	24	A	3.4
36	2e	12	LEU	3.4
40	2i	56	LEU	3.4
7	2H	124	GLU	3.4
7	2H	44	VAL	3.4
20	2Y	63	LYS	3.4
12	2Q	59	ARG	3.3
20	2Y	57	GLN	3.3
34	2c	200	ALA	3.3
39	2h	83	ILE	3.3
44	2m	7	VAL	3.3
48	2q	8	GLY	3.3
1	1A	931	C	3.3
33	2b	113	HIS	3.3
33	2b	24	TRP	3.3
39	2h	133	LEU	3.3
6	2G	160	VAL	3.3
35	1d	170	VAL	3.3
41	2j	10	GLY	3.3
19	2X	68	ARG	3.3
40	2i	121	ARG	3.3
7	2H	47	GLU	3.3
6	2G	17	PRO	3.3
33	2b	201	ILE	3.3
34	2c	180	ALA	3.3
41	2j	50	ILE	3.3
22	10	5	LYS	3.3
52	2u	6	ARG	3.3
45	2n	49	HIS	3.3
21	2Z	50	GLN	3.3
35	1d	157	LEU	3.3
7	2H	43	VAL	3.3
34	2c	21	ARG	3.3
1	1A	1142	A	3.3
47	2p	74	LEU	3.3
22	20	69	PHE	3.3
41	2j	54	PHE	3.3
22	10	3	HIS	3.3
43	2l	28	LYS	3.3
28	26	7	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
12	2Q	1	MET	3.3
34	1c	87	LEU	3.3
41	1j	60	ARG	3.3
21	2Z	174	VAL	3.3
26	24	7	PRO	3.3
6	2G	49	ASP	3.3
33	2b	36	ARG	3.3
34	1c	12	LEU	3.3
21	1Z	104	PHE	3.3
7	2H	35	VAL	3.3
38	2g	149	ARG	3.3
44	1m	87	TYR	3.2
6	2G	149	VAL	3.2
31	29	13	LYS	3.2
40	2i	53	VAL	3.2
41	2j	87	THR	3.2
26	14	46	GLN	3.2
44	2m	19	LEU	3.2
50	1s	71	LEU	3.2
50	2s	83	HIS	3.2
33	1b	188	ALA	3.2
35	2d	47	ARG	3.2
6	2G	26	GLN	3.2
36	2e	31	LEU	3.2
7	2H	17	VAL	3.2
34	2c	184	TYR	3.2
41	1j	10	GLY	3.2
49	1r	78	LEU	3.2
25	23	3	ARG	3.2
34	2c	172	ARG	3.2
47	2p	19	ILE	3.2
22	20	2	ALA	3.2
7	2H	131	VAL	3.2
11	2P	124	LYS	3.2
35	2d	184	LYS	3.2
20	2Y	65	ALA	3.2
43	2l	7	ILE	3.2
7	2H	141	VAL	3.2
26	14	50	VAL	3.2
41	2j	60	ARG	3.2
6	2G	138	GLN	3.2
34	2c	23	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
35	2d	186	LEU	3.2
6	2G	35	GLU	3.2
41	1j	46	ARG	3.1
34	2c	178	LEU	3.1
33	2b	79	ASP	3.1
33	2b	205	ASP	3.1
33	1b	126	GLU	3.1
34	2c	197	GLY	3.1
41	1j	8	LEU	3.1
3	2D	38	LYS	3.1
22	20	77	ARG	3.1
47	1p	4	ILE	3.1
46	2o	60	VAL	3.1
39	2h	128	GLY	3.1
34	2c	206	GLU	3.1
33	2b	163	PHE	3.1
6	2G	41	GLN	3.1
12	2Q	61	GLY	3.1
54	1w	20	U	3.1
22	20	3	HIS	3.1
40	2i	70	LYS	3.1
41	2j	56	HIS	3.1
50	2s	79	THR	3.1
5	2F	127	GLU	3.1
39	2h	2	LEU	3.1
21	2Z	148	ASP	3.1
40	1i	114	TYR	3.1
33	2b	235	SER	3.1
34	1c	39	ILE	3.1
47	1p	19	ILE	3.1
34	2c	145	GLY	3.1
52	2u	22	ARG	3.1
33	1b	75	LYS	3.1
12	1Q	33	GLY	3.1
44	2m	42	ALA	3.1
3	2D	111	LEU	3.1
1	2A	2896	C	3.1
54	2w	44	G	3.1
35	2d	161	ASN	3.1
34	2c	13	GLY	3.1
6	2G	181	ARG	3.1
40	2i	66	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
41	2j	61	GLU	3.1
42	2k	31	THR	3.1
40	2i	55	ALA	3.0
1	1A	1141	A	3.0
52	2u	15	ARG	3.0
28	26	50	ARG	3.0
43	2l	100	ILE	3.0
11	2P	125	VAL	3.0
11	2P	94	GLU	3.0
20	2Y	44	ILE	3.0
9	2N	23	LEU	3.0
12	2Q	65	PHE	3.0
40	1i	106	ALA	3.0
44	2m	12	ASN	3.0
26	24	42	PHE	3.0
35	2d	188	LEU	3.0
1	1A	2153	G	3.0
51	2t	55	ILE	3.0
6	1G	182	LYS	3.0
6	2G	73	ALA	3.0
11	2P	149	GLU	3.0
12	2Q	112	GLU	3.0
40	2i	106	ALA	3.0
25	23	26	LEU	3.0
32	1a	1531	A	3.0
40	2i	64	THR	3.0
33	2b	135	GLN	3.0
38	2g	6	ARG	3.0
30	28	63	PRO	3.0
35	2d	37	PRO	3.0
5	2F	12	LEU	3.0
26	14	52	THR	3.0
45	2n	51	GLY	3.0
6	2G	140	ILE	3.0
7	2H	167	GLU	3.0
6	2G	159	VAL	3.0
35	2d	185	PHE	2.9
44	2m	110	ARG	2.9
22	20	5	LYS	2.9
32	2a	1030	C	2.9
21	2Z	140	ASP	2.9
14	2S	14	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
3	1D	2	ALA	2.9
33	2b	120	ALA	2.9
6	2G	75	LYS	2.9
33	1b	27	LYS	2.9
38	2g	26	PHE	2.9
32	1a	1030	C	2.9
32	2a	1033	G	2.9
25	23	4	LEU	2.9
40	2i	21	PRO	2.9
44	2m	15	VAL	2.9
25	23	2	PRO	2.9
48	2q	100	LYS	2.9
47	1p	2	VAL	2.9
14	1S	48	LEU	2.9
1	1A	1140	U	2.9
1	2A	2154	G	2.9
38	2g	84	ASN	2.9
41	1j	98	ILE	2.9
7	1H	2	SER	2.9
11	2P	91	PHE	2.9
12	2Q	35	VAL	2.9
23	21	28	GLY	2.9
32	2a	1114	C	2.9
42	2k	14	VAL	2.9
48	2q	12	SER	2.9
6	2G	152	LEU	2.9
11	2P	45	LEU	2.9
40	2i	117	HIS	2.9
39	2h	94	TYR	2.9
48	2q	38	ARG	2.9
40	2i	54	ASP	2.9
3	2D	2	ALA	2.9
21	2Z	76	LEU	2.9
34	2c	163	ALA	2.9
38	2g	59	LEU	2.9
6	1G	181	ARG	2.9
1	2A	2155	G	2.9
5	2F	172	TRP	2.9
32	1a	841	U	2.9
21	2Z	156	LYS	2.9
7	2H	107	VAL	2.9
19	2X	13	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
6	2G	146	TYR	2.8
34	2c	8	ILE	2.8
6	2G	92	VAL	2.8
40	2i	128	ARG	2.8
46	2o	89	GLY	2.8
21	1Z	164	ALA	2.8
54	2w	31	A	2.8
54	2w	73	A	2.8
13	2R	69	ASP	2.8
40	1i	59	PHE	2.8
34	2c	28	GLN	2.8
1	2A	2319	G	2.8
54	2y	53	G	2.8
31	29	11	CYS	2.8
45	2n	29	ARG	2.8
1	2A	2133	G	2.8
6	2G	97	ASP	2.8
20	2Y	43	ASN	2.8
47	2p	76	GLN	2.8
14	2S	3	ARG	2.8
17	2V	73	SER	2.8
35	1d	110	PHE	2.8
6	1G	146	TYR	2.8
45	2n	53	LEU	2.8
12	2Q	38	GLU	2.8
42	1k	92	GLU	2.8
54	2y	65	G	2.8
3	1D	275	LYS	2.8
40	2i	116	LYS	2.8
33	2b	149	LEU	2.8
41	2j	85	LEU	2.8
9	2N	84	LYS	2.8
40	2i	87	GLN	2.8
42	2k	17	GLY	2.8
34	2c	199	LYS	2.8
35	2d	19	LEU	2.8
30	28	58	ILE	2.8
7	2H	132	ARG	2.8
41	2j	66	ARG	2.8
52	1u	17	THR	2.8
54	2y	35	A	2.7
38	1g	156	TRP	2.7

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Mol	Chain	Res	Type	RSRZ
33	1b	201	ILE	2.7
34	1c	8	ILE	2.7
40	2i	37	PHE	2.7
40	2i	95	LYS	2.7
1	2A	2127	G	2.7
32	2a	1001(A)	G	2.7
5	2F	167	ALA	2.7
7	2H	106	THR	2.7
33	2b	68	ILE	2.7
33	2b	69	LEU	2.7
33	2b	210	SER	2.7
34	2c	32	LEU	2.7
38	2g	86	GLN	2.7
5	2F	208	GLY	2.7
28	26	54	ILE	2.7
26	24	50	VAL	2.7
7	2H	84	SER	2.7
35	2d	175	SER	2.7
23	21	76	ARG	2.7
33	2b	226	ARG	2.7
24	22	1	MET	2.7
45	2n	22	THR	2.7
33	2b	42	ILE	2.7
40	1i	33	PHE	2.7
6	2G	47	LYS	2.7
9	2N	116	LEU	2.7
30	28	22	VAL	2.7
33	2b	71	VAL	2.7
33	2b	215	LEU	2.7
51	1t	36	LEU	2.7
51	2t	99	LEU	2.7
7	2H	97	ARG	2.7
21	2Z	51	ALA	2.7
14	2S	64	GLU	2.7
6	2G	88	ILE	2.7
6	2G	37	VAL	2.7
34	2c	183	ASP	2.7
38	1g	155	ARG	2.7
39	1h	61	VAL	2.7
48	2q	9	VAL	2.7
34	2c	149	ALA	2.7
1	1A	2154	U	2.7

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Mol	Chain	Res	Type	RSRZ
34	1c	128	PHE	2.7
7	2H	9	ILE	2.7
1	1A	2162	C	2.7
22	20	72	ARG	2.7
6	1G	152	LEU	2.7
54	2w	13	C	2.7
11	2P	122	PRO	2.7
33	2b	136	VAL	2.7
39	1h	78	GLN	2.7
39	2h	93	VAL	2.7
36	1e	95	ALA	2.7
7	2H	164	TYR	2.7
26	14	48	ARG	2.7
31	29	26	ILE	2.7
34	1c	126	ARG	2.7
9	2N	9	VAL	2.7
44	2m	93	ARG	2.7
45	1n	37	PHE	2.7
8	1I	79	ILE	2.7
38	2g	27	ILE	2.7
42	2k	32	ILE	2.7
42	2k	104	GLN	2.7
7	2H	52	VAL	2.7
7	2H	133	VAL	2.7
9	2N	122	VAL	2.7
44	2m	66	LEU	2.7
47	1p	49	LEU	2.7
22	10	4	LYS	2.7
22	20	80	HIS	2.7
35	2d	146	ILE	2.6
40	2i	77	ILE	2.6
14	2S	44	LYS	2.6
39	2h	116	LYS	2.6
51	1t	20	LEU	2.6
47	2p	79	VAL	2.6
11	2P	76	LYS	2.6
20	2Y	29	GLU	2.6
21	2Z	153	SER	2.6
32	2a	1030(C)	G	2.6
33	2b	63	MET	2.6
50	2s	35	SER	2.6
41	2j	49	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
12	2Q	33	GLY	2.6
7	2H	165	ALA	2.6
21	1Z	121	HIS	2.6
44	2m	92	HIS	2.6
48	2q	37	LYS	2.6
48	2q	87	LYS	2.6
8	2I	138	ILE	2.6
47	2p	51	VAL	2.6
6	2G	180	PHE	2.6
40	2i	124	GLN	2.6
21	2Z	154	ASP	2.6
49	2r	86	VAL	2.6
54	1y	56	C	2.6
36	1e	10	MET	2.6
39	2h	9	MET	2.6
47	2p	6	LEU	2.6
19	2X	69	TYR	2.6
6	2G	161	THR	2.6
33	2b	209	ARG	2.6
31	29	1	MET	2.6
34	2c	134	ILE	2.6
44	2m	78	ILE	2.6
47	1p	1	MET	2.6
14	2S	48	LEU	2.6
43	2l	72	GLY	2.6
54	2w	45	U	2.6
26	14	43	TYR	2.6
26	24	51	ASP	2.6
45	2n	59	ALA	2.6
8	1I	35	LEU	2.6
47	1p	32	TYR	2.6
38	2g	10	ARG	2.6
9	2N	43	THR	2.6
41	2j	6	ILE	2.6
45	2n	13	THR	2.6
7	2H	98	LEU	2.6
34	2c	148	GLY	2.6
20	2Y	7	VAL	2.6
39	2h	58	TYR	2.6
40	2i	83	ARG	2.6
44	2m	88	ARG	2.6
12	2Q	121	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
33	2b	28	PHE	2.6
23	21	68	PRO	2.6
21	2Z	146	ILE	2.5
24	12	70	GLN	2.5
26	24	31	ILE	2.5
8	2I	68	LEU	2.5
1	2A	886	C	2.5
12	2Q	22	LYS	2.5
20	2Y	4	LYS	2.5
27	25	57	VAL	2.5
54	1y	36	A	2.5
32	2a	1034	G	2.5
7	2H	96	ALA	2.5
33	2b	188	ALA	2.5
15	2T	48	ILE	2.5
7	2H	114	VAL	2.5
25	23	59	VAL	2.5
37	2f	59	TYR	2.5
1	1A	930	G	2.5
32	1a	1030(A)	G	2.5
35	2d	98	GLU	2.5
22	20	4	LYS	2.5
39	1h	83	ILE	2.5
14	2S	110	LEU	2.5
23	11	98	LEU	2.5
51	1t	72	LEU	2.5
33	2b	101	MET	2.5
12	1Q	32	TYR	2.5
33	2b	237	ALA	2.5
9	2N	11	PRO	2.5
51	2t	29	LYS	2.5
42	2k	66	LEU	2.5
33	2b	81	VAL	2.5
42	2k	87	THR	2.5
43	2l	55	VAL	2.5
49	2r	43	PHE	2.5
21	2Z	9	TYR	2.5
26	14	53	GLU	2.5
38	2g	83	ALA	2.5
47	2p	38	TYR	2.5
1	2A	887	A	2.5
33	2b	66	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
7	2H	162	ILE	2.5
6	2G	62	LEU	2.5
9	2N	26	LEU	2.5
51	1t	24	LEU	2.5
32	2a	1032	G	2.5
12	2Q	102	VAL	2.5
35	2d	112	VAL	2.5
40	1i	86	VAL	2.5
40	2i	105	ASP	2.5
26	14	32	TYR	2.5
26	24	45	GLY	2.5
12	2Q	64	ILE	2.5
34	2c	39	ILE	2.5
6	1G	135	LEU	2.5
33	2b	94	ASN	2.5
7	2H	24	VAL	2.5
7	2H	41	MET	2.5
22	20	45	PHE	2.5
33	2b	97	TRP	2.5
40	2i	4	TYR	2.5
1	2A	897	C	2.5
35	2d	169	LYS	2.5
15	2T	39	ARG	2.5
33	2b	59	GLU	2.5
35	2d	33	MET	2.5
34	2c	16	ARG	2.5
44	1m	2	ALA	2.5
47	1p	7	ALA	2.5
8	1I	109	ILE	2.5
25	23	53	LEU	2.5
40	2i	50	LEU	2.5
54	1w	3	C	2.5
7	2H	86	GLU	2.5
9	2N	74	ARG	2.5
25	13	60	GLU	2.5
19	2X	1	MET	2.5
32	2a	1030(D)	A	2.5
21	2Z	46	LYS	2.5
40	2i	30	GLY	2.5
43	2l	68	ALA	2.5
34	1c	89	GLU	2.4
45	2n	60	SER	2.4

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Mol	Chain	Res	Type	RSRZ
44	2m	103	THR	2.4
21	1Z	102	LEU	2.4
44	2m	104	ARG	2.4
51	1t	43	LEU	2.4
11	2P	78	PRO	2.4
1	1A	1106	U	2.4
40	2i	109	VAL	2.4
42	2k	109	VAL	2.4
26	24	54	GLY	2.4
1	1A	934	A	2.4
6	2G	19	LEU	2.4
35	2d	64	LEU	2.4
40	1i	110	GLU	2.4
33	2b	234	PRO	2.4
42	1k	81	ASP	2.4
41	2j	51	ARG	2.4
51	2t	59	ALA	2.4
47	2p	73	LEU	2.4
35	1d	138	TYR	2.4
5	2F	139	PHE	2.4
12	2Q	97	VAL	2.4
12	1Q	2	LEU	2.4
32	2a	1357	A	2.4
6	1G	80	PHE	2.4
15	2T	28	VAL	2.4
33	1b	165	VAL	2.4
36	2e	84	PHE	2.4
4	2E	2	LYS	2.4
7	2H	116	GLU	2.4
6	2G	43	LEU	2.4
33	2b	108	ILE	2.4
34	2c	188	LEU	2.4
39	2h	119	LEU	2.4
45	2n	7	ILE	2.4
46	1o	87	ILE	2.4
6	2G	122	PRO	2.4
7	2H	19	VAL	2.4
12	2Q	129	THR	2.4
19	2X	21	PHE	2.4
22	20	30	VAL	2.4
33	2b	130	ARG	2.4
35	2d	68	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
41	1j	48	THR	2.4
42	2k	91	ARG	2.4
54	1y	35	A	2.4
20	2Y	48	ALA	2.4
30	28	10	ALA	2.4
39	1h	63	LEU	2.4
1	2A	2125	G	2.4
20	2Y	42	VAL	2.4
40	2i	59	PHE	2.4
21	2Z	62	PRO	2.4
35	2d	27	TYR	2.4
40	2i	5	TYR	2.4
35	1d	70	ILE	2.4
38	2g	16	LEU	2.4
39	2h	86	ILE	2.4
38	1g	153	HIS	2.4
20	2Y	59	GLY	2.4
33	1b	228	GLY	2.4
42	2k	90	GLY	2.4
51	2t	18	GLN	2.4
1	1A	1144	A	2.4
40	2i	43	ALA	2.4
34	2c	124	ILE	2.4
39	2h	107	LEU	2.4
39	2h	122	ARG	2.4
40	2i	63	ILE	2.4
45	2n	47	LEU	2.4
45	2n	50	LYS	2.4
51	2t	30	LYS	2.4
8	2I	107	VAL	2.3
1	1A	2176	G	2.3
1	2A	2131	G	2.3
7	2H	23	ARG	2.3
12	1Q	59	ARG	2.3
22	20	74	ARG	2.3
23	21	69	LYS	2.3
6	1G	53	LEU	2.3
34	2c	111	LEU	2.3
52	1u	14	TRP	2.3
26	24	43	TYR	2.3
6	2G	155	MET	2.3
15	2T	40	THR	2.3

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Mol	Chain	Res	Type	RSRZ
14	2S	35	ILE	2.3
20	2Y	106	LEU	2.3
21	2Z	48	PHE	2.3
25	23	9	VAL	2.3
30	28	59	LYS	2.3
38	2g	9	VAL	2.3
40	1i	28	VAL	2.3
49	2r	21	LYS	2.3
21	1Z	99	TYR	2.3
32	2a	204	U	2.3
52	2u	21	TYR	2.3
20	2Y	36	ALA	2.3
40	2i	52	ALA	2.3
1	1A	2163	G	2.3
1	2A	2145	C	2.3
31	29	18	ARG	2.3
54	2w	4	C	2.3
25	23	29	ARG	2.3
44	1m	3	ARG	2.3
39	1h	79	VAL	2.3
32	2a	1202	G	2.3
8	1I	117	GLU	2.3
33	2b	33	TYR	2.3
6	1G	82	LEU	2.3
16	2U	98	LEU	2.3
33	2b	38	GLY	2.3
34	2c	185	GLY	2.3
40	2i	33	PHE	2.3
40	2i	73	GLN	2.3
14	2S	34	HIS	2.3
1	1A	1112	U	2.3
1	2A	1026	U	2.3
6	2G	36	LYS	2.3
40	1i	90	PRO	2.3
1	2A	652(U)	G	2.3
4	2E	151	TYR	2.3
29	27	1	MET	2.3
39	1h	62	TYR	2.3
34	1c	179	ARG	2.3
35	1d	158	ILE	2.3
11	2P	51	PHE	2.3
20	2Y	47	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
40	2i	123	PRO	2.3
8	2I	123	LEU	2.3
31	29	24	TYR	2.3
54	2y	61	C	2.3
38	1g	120	ILE	2.3
54	1w	44	G	2.3
25	23	7	LYS	2.3
16	2U	90	VAL	2.3
31	29	23	VAL	2.3
40	1i	65	VAL	2.3
44	2m	60	VAL	2.3
14	2S	30	ARG	2.3
44	2m	3	ARG	2.3
1	1A	933	C	2.3
7	2H	157	TYR	2.3
21	2Z	171	ILE	2.3
34	1c	124	ILE	2.3
34	1c	155	GLY	2.3
42	1k	50	TYR	2.3
52	1u	16	GLY	2.3
23	21	53	VAL	2.2
52	2u	5	ASP	2.2
4	2E	52	LEU	2.2
30	28	12	LYS	2.2
42	2k	15	ALA	2.2
34	1c	23	TYR	2.2
48	2q	95	TYR	2.2
25	23	38	GLU	2.2
11	2P	126	VAL	2.2
39	1h	93	VAL	2.2
45	1n	25	VAL	2.2
1	1A	1221	G	2.2
19	2X	88	LYS	2.2
34	1c	196	LEU	2.2
40	2i	80	GLY	2.2
47	1p	36	ILE	2.2
26	24	53	GLU	2.2
30	28	64	TYR	2.2
12	2Q	12	GLN	2.2
33	2b	184	VAL	2.2
34	2c	59	ARG	2.2
35	2d	140	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
38	1g	78	ARG	2.2
45	2n	41	ARG	2.2
11	2P	108	LYS	2.2
31	29	8	LYS	2.2
53	2v	12	A	2.2
54	2y	64	A	2.2
22	20	9	SER	2.2
14	2S	54	LEU	2.2
16	1U	4	ALA	2.2
33	2b	196	LEU	2.2
47	2p	1	MET	2.2
47	2p	80	PHE	2.2
6	2G	131	TYR	2.2
26	24	13	ARG	2.2
38	1g	18	TYR	2.2
40	1i	125	TYR	2.2
47	2p	48	TRP	2.2
1	1A	943	C	2.2
1	1A	2168	C	2.2
3	2D	59	LYS	2.2
22	20	51	VAL	2.2
44	1m	122	LYS	2.2
45	1n	50	LYS	2.2
45	1n	56	VAL	2.2
8	1I	72	LEU	2.2
19	2X	67	GLY	2.2
25	23	16	PRO	2.2
33	2b	32	ILE	2.2
36	2e	45	PHE	2.2
1	1A	2173	G	2.2
7	1H	6	ARG	2.2
32	2a	1031	G	2.2
42	2k	62	GLN	2.2
31	29	33	LYS	2.2
34	1c	201	TYR	2.2
43	2l	39	VAL	2.2
8	2I	122	GLU	2.2
34	2c	108	ASN	2.2
33	2b	51	LEU	2.2
41	2j	64	GLU	2.2
51	2t	20	LEU	2.2
8	2I	111	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
10	1O	47	ILE	2.2
39	1h	46	LYS	2.2
42	2k	108	ILE	2.2
34	1c	18	TRP	2.2
48	2q	21	VAL	2.2
6	2G	48	GLU	2.2
12	2Q	34	LEU	2.2
41	1j	5	ARG	2.2
20	2Y	38	ILE	2.2
20	2Y	75	ILE	2.2
15	2T	1	MET	2.2
1	2A	2156	G	2.2
22	20	73	GLY	2.2
39	2h	21	LYS	2.2
44	1m	91	ARG	2.2
54	2w	75	C	2.2
12	2Q	125	LEU	2.2
34	2c	91	LEU	2.2
51	1t	84	LEU	2.2
33	2b	218	ALA	2.2
34	2c	189	ALA	2.2
39	1h	134	ILE	2.2
11	2P	97	PRO	2.2
54	1w	76	A	2.2
22	20	78	TYR	2.2
38	1g	154	TYR	2.2
39	1h	48	TYR	2.2
40	1i	113	LYS	2.2
40	1i	8	GLY	2.2
45	2n	12	ARG	2.2
1	1A	1139	G	2.2
7	2H	123	PHE	2.2
21	1Z	155	LEU	2.2
48	1q	27	PHE	2.2
34	1c	134	ILE	2.2
36	1e	89	ILE	2.2
51	2t	33	ILE	2.2
52	1u	13	ILE	2.2
12	2Q	39	PRO	2.2
21	1Z	169	GLU	2.2
45	2n	58	LYS	2.2
35	2d	23	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
50	2s	52	TYR	2.2
20	2Y	60	PHE	2.1
42	1k	98	LEU	2.1
50	1s	16	LEU	2.1
45	1n	59	ALA	2.1
47	1p	48	TRP	2.1
6	2G	142	PRO	2.1
21	1Z	159	PRO	2.1
33	1b	226	ARG	2.1
33	2b	90	MET	2.1
52	1u	10	ARG	2.1
33	1b	227	GLY	2.1
40	2i	62	TYR	2.1
15	2T	22	PHE	2.1
33	1b	215	LEU	2.1
36	2e	119	LEU	2.1
41	1j	65	LEU	2.1
46	2o	57	LEU	2.1
15	2T	131	ALA	2.1
14	2S	10	ARG	2.1
22	20	82	ARG	2.1
40	2i	93	ARG	2.1
33	1b	26	PRO	2.1
1	1A	1105	G	2.1
15	2T	79	HIS	2.1
32	1a	1031	G	2.1
34	1c	64	VAL	2.1
48	2q	19	VAL	2.1
35	1d	207	TYR	2.1
4	2E	96	PHE	2.1
6	2G	135	LEU	2.1
20	2Y	28	LYS	2.1
23	21	46	LEU	2.1
40	2i	40	LEU	2.1
47	2p	35	LYS	2.1
6	1G	59	GLU	2.1
6	2G	63	ILE	2.1
7	2H	92	ILE	2.1
26	14	55	ARG	2.1
48	2q	92	ARG	2.1
35	2d	29	PRO	2.1
33	2b	57	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
40	2i	85	LEU	2.1
45	2n	44	LEU	2.1
47	2p	17	TYR	2.1
48	2q	42	TYR	2.1
36	2e	63	ARG	2.1
33	2b	208	ILE	2.1
35	2d	48	ALA	2.1
39	2h	13	ILE	2.1
32	1a	1030(D)	A	2.1
26	24	41	PRO	2.1
7	2H	76	VAL	2.1
51	2t	101	GLY	2.1
9	2N	12	ARG	2.1
14	2S	17	ARG	2.1
33	1b	64	ARG	2.1
34	2c	196	LEU	2.1
39	1h	10	LEU	2.1
39	1h	119	LEU	2.1
40	2i	51	ARG	2.1
45	2n	31	ARG	2.1
21	1Z	137	ILE	2.1
33	2b	127	ILE	2.1
40	1i	6	GLY	2.1
1	1A	2160	C	2.1
21	1Z	139	VAL	2.1
21	2Z	42	VAL	2.1
45	2n	33	VAL	2.1
33	2b	124	SER	2.1
40	1i	93	ARG	2.1
35	2d	162	LEU	2.1
39	1h	133	LEU	2.1
14	2S	92	TYR	2.1
19	2X	5	TYR	2.1
33	2b	78	GLN	2.1
39	1h	109	ILE	2.1
44	2m	9	ILE	2.1
40	1i	115	GLY	2.1
1	1A	1130	A	2.1
21	2Z	126	VAL	2.1
36	2e	14	ARG	2.1
36	2e	128	PRO	2.1
34	1c	101	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
41	1j	47	PHE	2.1
12	2Q	31	ASP	2.1
13	2R	21	TYR	2.1
17	2V	74	LYS	2.1
40	2i	112	LYS	2.1
19	2X	39	ILE	2.1
1	2A	881	G	2.1
8	1I	1	MET	2.1
50	2s	45	VAL	2.1
3	1D	38	LYS	2.1
21	2Z	151	HIS	2.1
33	2b	70	PHE	2.1
41	1j	63	PHE	2.1
8	2I	4	ILE	2.1
33	2b	160	ASP	2.1
22	10	2	ALA	2.1
30	28	29	LYS	2.1
47	2p	62	VAL	2.1
51	1t	81	LYS	2.1
5	2F	148	LEU	2.0
6	2G	103	LEU	2.0
11	1P	105	LEU	2.0
47	2p	49	LEU	2.0
23	21	65	SER	2.0
33	2b	216	SER	2.0
54	2w	2	C	2.0
1	2A	614(A)	U	2.0
21	2Z	172	ALA	2.0
26	24	68	ARG	2.0
31	29	19	ARG	2.0
35	1d	118	ARG	2.0
51	2t	41	ILE	2.0
14	1S	43	GLU	2.0
7	2H	29	PRO	2.0
7	2H	50	VAL	2.0
7	2H	144	VAL	2.0
35	2d	198	VAL	2.0
6	1G	19	LEU	2.0
6	2G	60	LEU	2.0
16	1U	117	GLN	2.0
41	2j	88	LEU	2.0
42	2k	93	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
17	2V	70	ILE	2.0
21	1Z	82	ARG	2.0
34	1c	14	ILE	2.0
34	2c	154	SER	2.0
37	1f	46	ARG	2.0
40	1i	51	ARG	2.0
10	2O	41	ALA	2.0
36	1e	94	ALA	2.0
37	1f	58	GLY	2.0
40	1i	46	ALA	2.0
43	1l	7	ILE	2.0
51	1t	41	ILE	2.0
18	2W	38	TYR	2.0
48	2q	7	THR	2.0
7	2H	128	PRO	2.0
16	2U	44	ASN	2.0
33	1b	234	PRO	2.0
12	2Q	17	LEU	2.0
35	1d	21	LEU	2.0
39	1h	112	LEU	2.0
47	2p	9	PHE	2.0
4	2E	124	GLY	2.0
21	2Z	57	ILE	2.0
50	1s	40	ILE	2.0
35	2d	117	ALA	2.0
26	24	25	TYR	2.0
54	1w	15	G	2.0
14	2S	5	THR	2.0
8	2I	1	MET	2.0
17	2V	5	VAL	2.0
34	1c	198	VAL	2.0
48	1q	35	VAL	2.0
9	2N	61	ARG	2.0
11	2P	79	ARG	2.0
19	2X	11	PRO	2.0
21	1Z	122	ARG	2.0
31	29	4	ARG	2.0
51	2t	25	ARG	2.0
47	1p	35	LYS	2.0
6	2G	39	ILE	2.0
9	2N	10	GLU	2.0
36	2e	114	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
49	2r	20	ALA	2.0
32	2a	1116	C	2.0
44	2m	23	TYR	2.0
1	1A	1114	G	2.0
22	20	63	VAL	2.0
36	2e	16	THR	2.0
53	2v	23	A	2.0
11	2P	1	MET	2.0
6	1G	133	LEU	2.0
7	2H	25	LYS	2.0
7	2H	33	LEU	2.0
11	2P	68	GLN	2.0
11	2P	88	LEU	2.0
18	1W	69	LEU	2.0
33	1b	95	GLN	2.0
40	1i	112	LYS	2.0
40	2i	47	LEU	2.0
51	1t	62	LEU	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	PSU	2y	55	20/21	0.68	0.22	102,113,127,129	0
54	4SU	2y	8	20/21	0.70	0.14	111,115,121,124	0
54	PSU	1y	55	20/21	0.74	0.29	101,108,115,126	0
54	7MG	2y	46	24/25	0.77	0.13	108,115,122,143	0
54	7MG	1w	46	24/25	0.77	0.18	88,103,119,135	0
54	7MG	2w	46	24/25	0.78	0.22	104,113,124,141	0
54	5MU	2y	54	21/22	0.78	0.29	100,108,120,137	0
54	MIA	2y	37	22/30	0.78	0.22	92,104,116,129	0
54	PSU	2y	32	20/21	0.79	0.26	99,110,119,121	0
54	4SU	2w	8	20/21	0.80	0.17	109,114,122,137	0
54	4SU	1y	8	20/21	0.81	0.16	101,107,113,113	0
54	4SU	1w	8	20/21	0.84	0.18	91,99,107,109	0
54	PSU	2w	55	20/21	0.85	0.21	92,97,106,108	0
55	4SU	2x	8	20/21	0.85	0.22	77,88,93,93	0
55	PSU	2x	55	20/21	0.86	0.15	80,89,100,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	PSU	1w	55	20/21	0.86	0.18	70,90,98,99	0
54	PSU	2y	39	20/21	0.86	0.18	91,101,110,111	0
54	7MG	1y	46	24/25	0.88	0.27	101,112,119,130	0
54	5MU	1y	54	21/22	0.88	0.33	97,103,113,129	0
54	PSU	1y	39	20/21	0.88	0.17	85,91,104,106	0
54	PSU	2w	39	20/21	0.89	0.26	82,94,99,99	0
54	PSU	1y	32	20/21	0.89	0.16	84,92,101,101	0
54	MIA	1y	37	22/30	0.91	0.12	81,90,97,99	0
32	2MG	2a	1207	24/25	0.92	0.13	86,91,99,102	0
54	PSU	2w	32	20/21	0.92	0.25	87,95,100,102	0
32	5MC	2a	967	21/22	0.93	0.19	78,81,86,94	0
54	MIA	2w	37	25/30	0.93	0.19	79,89,94,97	0
55	4SU	1x	8	20/21	0.93	0.19	60,68,78,79	0
32	5MC	2a	1400	21/22	0.93	0.26	72,81,85,92	0
54	5MU	2w	54	21/22	0.93	0.13	79,91,95,99	0
32	5MC	2a	1407	21/22	0.93	0.19	60,65,71,82	0
32	PSU	2a	516	20/21	0.93	0.13	76,83,89,89	0
55	5MC	2x	32	21/22	0.93	0.21	75,83,87,88	0
54	PSU	1w	32	20/21	0.94	0.13	68,78,82,83	0
55	5MU	2x	54	21/22	0.94	0.15	88,93,99,109	0
1	5MU	1A	1937	21/22	0.94	0.19	56,63,70,74	0
32	7MG	2a	527	24/25	0.94	0.19	66,72,78,82	0
32	M2G	2a	966	25/26	0.94	0.19	68,79,87,92	0
32	4OC	2a	1402	22/23	0.95	0.15	64,71,75,78	0
55	PSU	1x	55	20/21	0.95	0.13	66,70,78,83	0
32	MA6	2a	1519	24/25	0.95	0.24	57,69,76,82	0
54	5MU	1w	54	21/22	0.95	0.18	62,76,84,85	0
1	PSU	2A	1917	20/21	0.95	0.16	72,78,88,88	0
1	5MC	2A	1962	21/22	0.95	0.26	50,57,68,78	0
55	5MU	1x	54	21/22	0.95	0.14	64,75,79,84	0
1	4OC	2A	1920	21/23	0.96	0.17	67,72,75,78	0
1	5MC	2A	1942	21/22	0.96	0.21	56,70,78,85	0
32	5MC	2a	1404	21/22	0.96	0.15	54,63,68,70	0
54	MIA	1w	37	29/30	0.96	0.17	51,58,69,70	0
32	UR3	2a	1498	21/22	0.96	0.19	60,64,69,78	0
32	MA6	2a	1518	24/25	0.96	0.19	54,70,74,77	0
1	PSU	2A	2605	20/21	0.96	0.20	34,47,51,52	0
43	0TD	2l	92	10/11	0.96	0.21	64,69,74,81	0
54	PSU	1w	39	20/21	0.96	0.17	53,72,76,78	0
32	PSU	1a	516	20/21	0.96	0.15	54,64,71,71	0
1	PSU	2A	1911	20/21	0.96	0.17	66,72,75,75	0
1	5MU	2A	1915	21/22	0.96	0.16	76,83,88,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	7MG	1a	527	24/25	0.96	0.18	47,53,57,59	0
1	PSU	1A	1933	20/21	0.97	0.17	44,51,56,58	0
1	PSU	1A	1939	20/21	0.97	0.17	40,57,64,66	0
32	M2G	1a	966	25/26	0.97	0.18	56,61,69,70	0
1	OMG	2A	2251	24/25	0.97	0.21	45,51,56,60	0
1	2MA	2A	2503	23/24	0.97	0.21	34,44,50,54	0
1	2MU	2A	2552	21/23	0.97	0.19	40,45,56,62	0
55	5MC	1x	32	21/22	0.97	0.18	52,57,62,65	0
32	5MC	1a	967	21/22	0.97	0.20	57,63,68,70	0
32	2MG	1a	1207	24/25	0.97	0.12	54,70,73,76	0
32	5MC	1a	1400	21/22	0.97	0.20	43,54,62,67	0
32	5MC	1a	1404	21/22	0.97	0.19	42,46,51,51	0
32	MA6	1a	1518	24/25	0.97	0.23	40,48,52,58	0
32	MA6	1a	1519	24/25	0.97	0.22	43,48,53,58	0
43	0TD	1l	92	10/11	0.97	0.15	48,51,54,65	0
1	5MU	1A	1961	21/22	0.97	0.23	36,39,43,51	0
1	5MC	1A	1964	21/22	0.97	0.17	46,50,55,56	0
1	OMG	1A	2263	24/25	0.97	0.20	24,30,34,38	0
1	2MU	1A	2564	21/23	0.97	0.19	31,36,40,44	0
1	PSU	1A	2617	20/21	0.97	0.22	24,35,39,40	0
1	2MA	1A	2515	23/24	0.98	0.17	21,27,32,34	0
32	5MC	1a	1407	21/22	0.98	0.19	40,46,50,53	0
32	UR3	1a	1498	21/22	0.98	0.20	34,45,49,55	0
1	5MC	1A	1984	21/22	0.98	0.20	31,45,47,49	0
1	5MU	2A	1939	21/22	0.98	0.21	47,51,55,58	0
1	4OC	1A	1942	21/23	0.98	0.21	41,49,55,56	0
32	4OC	1a	1402	22/23	0.98	0.18	46,53,58,68	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(Å^2)	Q<0.9
56	MG	2A	3110	1/1	0.12	0.16	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3202	1/1	0.23	0.55	74,74,74,74	0
56	MG	2v	102	1/1	0.24	0.36	89,89,89,89	0
56	MG	2a	1664	1/1	0.25	0.12	89,89,89,89	0
56	MG	2A	3456	1/1	0.26	1.22	97,97,97,97	0
56	MG	1B	220	1/1	0.27	0.47	81,81,81,81	0
56	MG	2A	3498	1/1	0.28	0.25	90,90,90,90	0
56	MG	1x	123	1/1	0.35	0.33	85,85,85,85	0
56	MG	1A	3784	1/1	0.36	0.49	76,76,76,76	0
56	MG	2A	3255	1/1	0.37	0.34	76,76,76,76	0
56	MG	1A	3029	1/1	0.39	0.90	63,63,63,63	0
56	MG	1a	1832	1/1	0.42	0.28	78,78,78,78	0
56	MG	2A	3442	1/1	0.42	0.14	78,78,78,78	0
56	MG	1A	3865	1/1	0.44	0.21	79,79,79,79	0
56	MG	2A	3291	1/1	0.44	0.36	82,82,82,82	0
56	MG	2A	3333	1/1	0.44	0.64	79,79,79,79	0
56	MG	1a	1872	1/1	0.44	0.19	71,71,71,71	0
56	MG	1A	3730	1/1	0.45	0.17	73,73,73,73	0
56	MG	2A	3327	1/1	0.45	0.28	86,86,86,86	0
56	MG	1A	3856	1/1	0.46	0.41	70,70,70,70	0
56	MG	1A	3838	1/1	0.46	0.25	84,84,84,84	0
56	MG	1a	1680	1/1	0.47	0.16	83,83,83,83	0
56	MG	1A	3085	1/1	0.47	0.23	73,73,73,73	0
56	MG	1y	101	1/1	0.47	0.39	66,66,66,66	0
56	MG	2a	1725	1/1	0.47	0.41	96,96,96,96	0
56	MG	2A	3451	1/1	0.47	0.46	84,84,84,84	0
56	MG	1A	3770	1/1	0.48	0.40	74,74,74,74	0
56	MG	2A	3496	1/1	0.48	1.11	91,91,91,91	0
56	MG	1a	1609	1/1	0.49	0.62	81,81,81,81	0
56	MG	1Q	203	1/1	0.49	0.15	63,63,63,63	0
56	MG	2A	3517	1/1	0.49	0.25	91,91,91,91	0
56	MG	23	101	1/1	0.50	0.67	73,73,73,73	0
56	MG	1A	3873	1/1	0.51	0.17	52,52,52,52	0
56	MG	2A	3360	1/1	0.51	0.52	77,77,77,77	0
56	MG	2a	1698	1/1	0.52	0.31	86,86,86,86	0
56	MG	1A	3387	1/1	0.52	0.26	74,74,74,74	0
56	MG	1a	1890	1/1	0.52	0.12	83,83,83,83	0
56	MG	1A	3887	1/1	0.53	0.37	61,61,61,61	0
56	MG	1a	1763	1/1	0.53	0.15	73,73,73,73	0
56	MG	1a	1831	1/1	0.54	0.15	102,102,102,102	0
56	MG	1A	3920	1/1	0.54	0.29	95,95,95,95	0
56	MG	2a	1803	1/1	0.54	0.21	82,82,82,82	0
56	MG	1a	1847	1/1	0.54	0.22	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	1605	1/1	0.55	0.69	73,73,73,73	0
56	MG	2B	206	1/1	0.55	0.23	73,73,73,73	0
56	MG	1A	3668	1/1	0.55	0.31	69,69,69,69	0
56	MG	2a	1613	1/1	0.56	0.23	81,81,81,81	0
56	MG	1A	3604	1/1	0.56	0.18	71,71,71,71	0
56	MG	2a	1685	1/1	0.56	0.24	81,81,81,81	0
56	MG	1a	1883	1/1	0.56	1.16	89,89,89,89	0
56	MG	1A	3929	1/1	0.56	0.67	69,69,69,69	0
56	MG	1A	3900	1/1	0.56	0.13	75,75,75,75	0
56	MG	1a	1691	1/1	0.56	0.14	75,75,75,75	0
56	MG	1a	1912	1/1	0.57	0.48	71,71,71,71	0
56	MG	2a	1797	1/1	0.57	0.25	99,99,99,99	0
56	MG	2A	3524	1/1	0.57	0.86	79,79,79,79	0
56	MG	1A	3881	1/1	0.57	0.26	62,62,62,62	0
56	MG	2A	3448	1/1	0.58	0.21	71,71,71,71	0
56	MG	2A	3287	1/1	0.58	0.34	60,60,60,60	0
56	MG	1A	3853	1/1	0.58	0.14	59,59,59,59	0
56	MG	2A	3414	1/1	0.58	0.21	55,55,55,55	0
56	MG	2a	1730	1/1	0.58	0.70	83,83,83,83	0
56	MG	1A	3124	1/1	0.58	0.29	56,56,56,56	0
56	MG	2a	1611	1/1	0.58	0.39	80,80,80,80	0
56	MG	2a	1827	1/1	0.58	0.11	74,74,74,74	0
56	MG	2A	3510	1/1	0.58	0.30	87,87,87,87	0
56	MG	1A	3168	1/1	0.59	0.97	81,81,81,81	0
56	MG	1a	1615	1/1	0.59	0.62	83,83,83,83	0
56	MG	2A	3441	1/1	0.59	0.29	85,85,85,85	0
56	MG	2A	3500	1/1	0.59	0.13	80,80,80,80	0
56	MG	1A	3615	1/1	0.59	0.43	50,50,50,50	0
56	MG	1B	228	1/1	0.59	0.33	80,80,80,80	0
56	MG	1A	3175	1/1	0.59	0.24	83,83,83,83	0
56	MG	1a	1882	1/1	0.60	0.06	86,86,86,86	0
56	MG	1A	3388	1/1	0.60	0.28	74,74,74,74	0
56	MG	2T	202	1/1	0.60	0.62	82,82,82,82	0
56	MG	1A	3558	1/1	0.60	0.70	58,58,58,58	0
56	MG	1A	3845	1/1	0.61	0.73	65,65,65,65	0
56	MG	1A	3658	1/1	0.61	0.41	66,66,66,66	0
56	MG	1a	1936	1/1	0.61	0.26	71,71,71,71	0
56	MG	1q	202	1/1	0.61	0.12	76,76,76,76	0
56	MG	1A	3793	1/1	0.62	0.39	65,65,65,65	0
56	MG	1A	3638	1/1	0.62	0.17	73,73,73,73	0
56	MG	2A	3560	1/1	0.62	0.32	82,82,82,82	0
56	MG	1A	3606	1/1	0.62	0.32	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	1623	1/1	0.62	0.21	70,70,70,70	0
56	MG	2A	3130	1/1	0.62	0.30	73,73,73,73	0
56	MG	21	101	1/1	0.62	0.39	82,82,82,82	0
56	MG	1A	3850	1/1	0.63	0.44	59,59,59,59	0
56	MG	1a	1855	1/1	0.63	0.20	63,63,63,63	0
56	MG	2A	3329	1/1	0.63	0.24	86,86,86,86	0
56	MG	2a	1773	1/1	0.63	0.45	91,91,91,91	0
56	MG	1A	3151	1/1	0.63	0.18	68,68,68,68	0
56	MG	2a	1800	1/1	0.63	0.28	86,86,86,86	0
56	MG	2A	3144	1/1	0.63	0.10	91,91,91,91	0
56	MG	1A	3402	1/1	0.63	0.43	63,63,63,63	0
56	MG	1A	3167	1/1	0.63	0.76	46,46,46,46	0
56	MG	2A	3128	1/1	0.64	0.33	73,73,73,73	0
56	MG	1a	1674	1/1	0.64	0.18	78,78,78,78	0
56	MG	2A	3134	1/1	0.64	0.18	69,69,69,69	0
56	MG	1A	3772	1/1	0.64	0.25	76,76,76,76	0
56	MG	1A	3165	1/1	0.64	0.70	52,52,52,52	0
56	MG	2B	209	1/1	0.64	0.10	76,76,76,76	0
56	MG	1A	3464	1/1	0.65	0.21	83,83,83,83	0
56	MG	1o	102	1/1	0.65	0.15	76,76,76,76	0
56	MG	1a	1889	1/1	0.65	0.23	75,75,75,75	0
56	MG	1a	1915	1/1	0.65	0.12	85,85,85,85	0
56	MG	2A	3447	1/1	0.65	0.68	86,86,86,86	0
56	MG	1a	1693	1/1	0.66	0.14	63,63,63,63	0
56	MG	2A	3545	1/1	0.66	0.17	72,72,72,72	0
56	MG	1A	3751	1/1	0.66	0.35	72,72,72,72	0
56	MG	1A	3653	1/1	0.66	0.16	84,84,84,84	0
56	MG	1A	3195	1/1	0.66	0.27	68,68,68,68	0
56	MG	2F	301	1/1	0.66	0.34	63,63,63,63	0
56	MG	1A	3139	1/1	0.66	0.37	68,68,68,68	0
56	MG	1A	3384	1/1	0.66	0.28	72,72,72,72	0
56	MG	2A	3422	1/1	0.67	0.29	57,57,57,57	0
56	MG	1A	3792	1/1	0.67	0.89	78,78,78,78	0
56	MG	2A	3520	1/1	0.67	0.26	59,59,59,59	0
56	MG	2A	3345	1/1	0.67	0.16	69,69,69,69	0
56	MG	2A	3061	1/1	0.67	0.60	79,79,79,79	0
56	MG	2a	1825	1/1	0.67	0.13	58,58,58,58	0
56	MG	1A	3922	1/1	0.67	0.20	67,67,67,67	0
56	MG	2A	3563	1/1	0.67	0.16	78,78,78,78	0
56	MG	1a	1948	1/1	0.68	0.07	69,69,69,69	0
56	MG	1a	1854	1/1	0.68	0.21	83,83,83,83	0
56	MG	1a	1918	1/1	0.68	0.34	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1a	1924	1/1	0.68	0.64	83,83,83,83	0
56	MG	2a	1775	1/1	0.68	0.11	73,73,73,73	0
56	MG	1A	3644	1/1	0.68	0.27	57,57,57,57	0
56	MG	2A	3332	1/1	0.68	1.67	80,80,80,80	0
56	MG	2a	1663	1/1	0.68	0.22	85,85,85,85	0
56	MG	2A	3027	1/1	0.68	0.28	58,58,58,58	0
56	MG	2a	1667	1/1	0.68	0.10	81,81,81,81	0
56	MG	2A	3340	1/1	0.68	0.09	69,69,69,69	0
56	MG	1A	3761	1/1	0.69	0.63	79,79,79,79	0
56	MG	1A	3083	1/1	0.69	0.19	71,71,71,71	0
56	MG	1A	3218	1/1	0.69	0.52	75,75,75,75	0
56	MG	1A	3196	1/1	0.69	0.48	62,62,62,62	0
56	MG	2a	1679	1/1	0.69	0.41	73,73,73,73	0
56	MG	1a	1934	1/1	0.69	0.39	57,57,57,57	0
56	MG	2a	1822	1/1	0.69	0.31	71,71,71,71	0
56	MG	2a	1686	1/1	0.69	0.24	80,80,80,80	0
56	MG	1a	1618	1/1	0.69	0.51	75,75,75,75	0
56	MG	1a	1942	1/1	0.69	0.19	79,79,79,79	0
56	MG	1a	1738	1/1	0.70	0.13	95,95,95,95	0
56	MG	2a	1705	1/1	0.70	0.56	79,79,79,79	0
56	MG	1a	1746	1/1	0.70	0.21	85,85,85,85	0
56	MG	2A	3529	1/1	0.70	0.28	82,82,82,82	0
56	MG	2A	3342	1/1	0.70	0.27	77,77,77,77	0
56	MG	1a	1878	1/1	0.70	0.14	77,77,77,77	0
56	MG	2a	1662	1/1	0.70	0.17	73,73,73,73	0
56	MG	2A	3495	1/1	0.70	0.16	74,74,74,74	0
56	MG	1A	3002	1/1	0.70	0.23	66,66,66,66	0
56	MG	1A	3187	1/1	0.70	0.64	81,81,81,81	0
56	MG	1A	3915	1/1	0.70	0.23	86,86,86,86	0
56	MG	1A	3229	1/1	0.70	0.40	63,63,63,63	0
56	MG	1a	1713	1/1	0.70	0.54	75,75,75,75	0
56	MG	1a	1800	1/1	0.71	0.27	80,80,80,80	0
56	MG	2a	1699	1/1	0.71	0.33	81,81,81,81	0
56	MG	2A	3526	1/1	0.71	0.16	76,76,76,76	0
56	MG	2a	1723	1/1	0.71	0.09	84,84,84,84	0
56	MG	1A	3716	1/1	0.71	0.21	63,63,63,63	0
56	MG	1A	3422	1/1	0.71	0.59	61,61,61,61	0
56	MG	2A	3547	1/1	0.71	0.29	81,81,81,81	0
56	MG	2a	1644	1/1	0.71	0.12	83,83,83,83	0
56	MG	2a	1785	1/1	0.71	0.21	60,60,60,60	0
56	MG	1a	1712	1/1	0.71	0.29	69,69,69,69	0
56	MG	1w	104	1/1	0.71	0.72	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3190	1/1	0.71	0.25	55,55,55,55	0
56	MG	1A	3403	1/1	0.71	0.45	56,56,56,56	0
56	MG	1A	3559	1/1	0.71	0.29	54,54,54,54	0
56	MG	1B	229	1/1	0.71	0.25	68,68,68,68	0
56	MG	1a	1785	1/1	0.71	0.11	64,64,64,64	0
56	MG	2A	3341	1/1	0.72	0.13	81,81,81,81	0
56	MG	1A	3129	1/1	0.72	0.25	83,83,83,83	0
56	MG	1A	3091	1/1	0.72	0.23	64,64,64,64	0
56	MG	1v	103	1/1	0.72	0.29	79,79,79,79	0
56	MG	2A	3459	1/1	0.72	0.25	56,56,56,56	0
56	MG	2A	3543	1/1	0.72	0.36	88,88,88,88	0
56	MG	2A	3379	1/1	0.72	0.23	59,59,59,59	0
56	MG	1A	3868	1/1	0.72	0.20	83,83,83,83	0
56	MG	1A	3227	1/1	0.72	0.61	54,54,54,54	0
56	MG	1A	3140	1/1	0.72	0.11	71,71,71,71	0
56	MG	1A	3252	1/1	0.72	0.47	67,67,67,67	0
56	MG	2a	1712	1/1	0.73	0.09	74,74,74,74	0
56	MG	1A	3409	1/1	0.73	0.15	69,69,69,69	0
56	MG	2A	3565	1/1	0.73	0.17	64,64,64,64	0
56	MG	2A	3163	1/1	0.73	0.36	76,76,76,76	0
56	MG	2a	1738	1/1	0.73	0.17	75,75,75,75	0
56	MG	1A	3744	1/1	0.73	0.35	72,72,72,72	0
56	MG	1a	1778	1/1	0.73	0.23	53,53,53,53	0
56	MG	2G	201	1/1	0.73	0.09	75,75,75,75	0
56	MG	1a	1950	1/1	0.73	0.26	92,92,92,92	0
56	MG	1a	1671	1/1	0.73	0.30	69,69,69,69	0
56	MG	2a	1801	1/1	0.73	0.40	75,75,75,75	0
56	MG	2A	3391	1/1	0.73	0.35	78,78,78,78	0
56	MG	19	101	1/1	0.73	0.18	70,70,70,70	0
56	MG	1a	1725	1/1	0.73	0.10	76,76,76,76	0
56	MG	2a	1700	1/1	0.73	0.11	77,77,77,77	0
56	MG	1A	3908	1/1	0.73	0.17	61,61,61,61	0
56	MG	2A	3505	1/1	0.74	0.23	82,82,82,82	0
56	MG	20	102	1/1	0.74	0.53	68,68,68,68	0
56	MG	2A	3408	1/1	0.74	0.38	58,58,58,58	0
56	MG	1A	3610	1/1	0.74	0.14	54,54,54,54	0
56	MG	1A	3931	1/1	0.74	0.14	74,74,74,74	0
56	MG	2A	3433	1/1	0.74	0.47	51,51,51,51	0
56	MG	1A	3855	1/1	0.74	0.18	69,69,69,69	0
56	MG	1a	1863	1/1	0.74	0.13	80,80,80,80	0
56	MG	1A	3837	1/1	0.74	0.52	51,51,51,51	0
56	MG	1A	3121	1/1	0.74	0.63	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1a	1782	1/1	0.74	0.07	81,81,81,81	0
56	MG	1A	3757	1/1	0.74	0.31	65,65,65,65	0
56	MG	18	102	1/1	0.74	0.22	55,55,55,55	0
56	MG	2A	3471	1/1	0.74	0.29	78,78,78,78	0
56	MG	1A	3149	1/1	0.74	0.21	70,70,70,70	0
56	MG	1a	1892	1/1	0.74	0.10	68,68,68,68	0
56	MG	1A	3875	1/1	0.74	0.19	72,72,72,72	0
56	MG	2A	3401	1/1	0.74	0.32	59,59,59,59	0
56	MG	1A	3595	1/1	0.75	0.31	51,51,51,51	0
56	MG	2A	3028	1/1	0.75	0.31	57,57,57,57	0
56	MG	2A	3038	1/1	0.75	0.43	57,57,57,57	0
56	MG	2A	3461	1/1	0.75	0.12	58,58,58,58	0
56	MG	1A	3601	1/1	0.75	0.20	43,43,43,43	0
56	MG	2B	210	1/1	0.75	0.16	74,74,74,74	0
56	MG	2B	211	1/1	0.75	0.36	90,90,90,90	0
56	MG	2A	3481	1/1	0.75	0.22	71,71,71,71	0
56	MG	1A	3247	1/1	0.75	0.17	68,68,68,68	0
56	MG	1A	3166	1/1	0.75	0.56	58,58,58,58	0
56	MG	1a	1769	1/1	0.75	0.85	79,79,79,79	0
56	MG	2A	3387	1/1	0.75	0.19	73,73,73,73	0
56	MG	1A	3803	1/1	0.75	0.30	55,55,55,55	0
56	MG	1A	3358	1/1	0.75	0.47	62,62,62,62	0
56	MG	1e	201	1/1	0.75	0.94	77,77,77,77	0
56	MG	2A	3229	1/1	0.75	0.14	72,72,72,72	0
56	MG	2a	1621	1/1	0.75	0.09	99,99,99,99	0
56	MG	1A	3371	1/1	0.75	0.35	60,60,60,60	0
56	MG	1A	3138	1/1	0.75	0.42	65,65,65,65	0
56	MG	2a	1813	1/1	0.75	0.11	90,90,90,90	0
56	MG	1A	3010	1/1	0.75	0.22	66,66,66,66	0
56	MG	1a	1901	1/1	0.75	0.32	76,76,76,76	0
56	MG	10	101	1/1	0.75	0.44	46,46,46,46	0
56	MG	1A	3137	1/1	0.75	0.31	70,70,70,70	0
56	MG	1a	1611	1/1	0.76	0.22	64,64,64,64	0
56	MG	2A	3530	1/1	0.76	0.17	74,74,74,74	0
56	MG	1A	3432	1/1	0.76	0.19	56,56,56,56	0
56	MG	1a	1730	1/1	0.76	0.16	76,76,76,76	0
56	MG	2A	3546	1/1	0.76	0.18	70,70,70,70	0
56	MG	1a	1737	1/1	0.76	0.25	89,89,89,89	0
56	MG	2A	3557	1/1	0.76	0.33	62,62,62,62	0
56	MG	1A	3282	1/1	0.76	0.36	44,44,44,44	0
56	MG	1a	1923	1/1	0.76	0.28	81,81,81,81	0
56	MG	1A	3003	1/1	0.76	0.24	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3673	1/1	0.76	0.13	43,43,43,43	0
56	MG	1A	3142	1/1	0.76	0.34	60,60,60,60	0
56	MG	2a	1802	1/1	0.76	0.18	81,81,81,81	0
56	MG	1a	1777	1/1	0.76	0.27	71,71,71,71	0
56	MG	2A	3513	1/1	0.76	0.64	82,82,82,82	0
56	MG	1A	3146	1/1	0.76	0.22	69,69,69,69	0
56	MG	1A	3878	1/1	0.76	0.22	57,57,57,57	0
56	MG	1A	3023	1/1	0.76	0.20	55,55,55,55	0
56	MG	1a	1792	1/1	0.76	0.45	59,59,59,59	0
56	MG	2a	1771	1/1	0.77	0.11	82,82,82,82	0
56	MG	2A	3509	1/1	0.77	0.22	57,57,57,57	0
56	MG	1a	1745	1/1	0.77	0.94	71,71,71,71	0
56	MG	2a	1778	1/1	0.77	0.17	87,87,87,87	0
56	MG	1A	3331	1/1	0.77	0.35	55,55,55,55	0
56	MG	1A	3208	1/1	0.77	0.18	84,84,84,84	0
56	MG	1a	1879	1/1	0.77	0.09	87,87,87,87	0
56	MG	2A	3361	1/1	0.77	0.26	67,67,67,67	0
56	MG	2B	202	1/1	0.77	0.22	68,68,68,68	0
56	MG	2A	3377	1/1	0.77	0.30	59,59,59,59	0
56	MG	2a	1807	1/1	0.77	0.15	79,79,79,79	0
56	MG	14	502	1/1	0.77	0.28	79,79,79,79	0
56	MG	1A	3701	1/1	0.77	0.08	42,42,42,42	0
56	MG	2A	3532	1/1	0.77	0.98	64,64,64,64	0
56	MG	1a	1947	1/1	0.77	0.17	81,81,81,81	0
56	MG	2A	3395	1/1	0.77	0.29	50,50,50,50	0
56	MG	1A	3253	1/1	0.78	0.15	73,73,73,73	0
56	MG	1A	3886	1/1	0.78	0.37	39,39,39,39	0
56	MG	2Q	202	1/1	0.78	0.37	75,75,75,75	0
56	MG	1a	1774	1/1	0.78	0.12	76,76,76,76	0
56	MG	2A	3043	1/1	0.78	0.25	53,53,53,53	0
56	MG	1A	3706	1/1	0.78	0.20	55,55,55,55	0
56	MG	1A	3154	1/1	0.78	0.40	67,67,67,67	0
56	MG	1A	3436	1/1	0.78	0.28	57,57,57,57	0
56	MG	2A	3353	1/1	0.78	0.11	81,81,81,81	0
56	MG	1A	3299	1/1	0.78	0.55	57,57,57,57	0
56	MG	1A	3866	1/1	0.78	0.34	69,69,69,69	0
56	MG	2A	3368	1/1	0.78	0.19	80,80,80,80	0
56	MG	1a	1795	1/1	0.78	0.14	55,55,55,55	0
56	MG	2A	3159	1/1	0.78	0.46	69,69,69,69	0
56	MG	1A	3749	1/1	0.78	0.17	66,66,66,66	0
56	MG	1a	1899	1/1	0.78	0.07	77,77,77,77	0
56	MG	1A	3660	1/1	0.78	0.20	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	1678	1/1	0.78	0.49	72,72,72,72	0
56	MG	2B	203	1/1	0.78	0.14	75,75,75,75	0
56	MG	2A	3399	1/1	0.78	0.36	41,41,41,41	0
56	MG	1A	3617	1/1	0.78	0.33	50,50,50,50	0
56	MG	1B	205	1/1	0.78	0.25	50,50,50,50	0
56	MG	1A	3630	1/1	0.78	0.18	78,78,78,78	0
56	MG	1A	3665	1/1	0.79	0.14	59,59,59,59	0
56	MG	2A	3428	1/1	0.79	0.19	78,78,78,78	0
56	MG	1A	3410	1/1	0.79	0.17	72,72,72,72	0
56	MG	19	102	1/1	0.79	0.27	55,55,55,55	0
56	MG	1A	3637	1/1	0.79	0.32	61,61,61,61	0
56	MG	1A	3418	1/1	0.79	0.33	55,55,55,55	0
56	MG	1a	1857	1/1	0.79	0.18	71,71,71,71	0
56	MG	2a	1740	1/1	0.79	0.27	58,58,58,58	0
56	MG	2A	3075	1/1	0.79	0.38	81,81,81,81	0
56	MG	1B	203	1/1	0.79	0.24	74,74,74,74	0
56	MG	1A	3641	1/1	0.79	0.25	66,66,66,66	0
56	MG	1A	3538	1/1	0.79	0.30	53,53,53,53	0
56	MG	2a	1782	1/1	0.79	0.43	65,65,65,65	0
56	MG	1B	223	1/1	0.79	0.14	63,63,63,63	0
56	MG	2a	1655	1/1	0.79	0.26	72,72,72,72	0
56	MG	1A	3421	1/1	0.79	0.25	61,61,61,61	0
56	MG	2A	3484	1/1	0.79	0.28	67,67,67,67	0
56	MG	1a	1779	1/1	0.79	0.23	68,68,68,68	0
56	MG	1A	3891	1/1	0.79	0.17	69,69,69,69	0
56	MG	1D	302	1/1	0.79	0.46	57,57,57,57	0
56	MG	1A	3862	1/1	0.79	0.29	70,70,70,70	0
56	MG	1w	103	1/1	0.79	0.26	81,81,81,81	0
56	MG	2A	3290	1/1	0.79	0.12	55,55,55,55	0
56	MG	1A	3032	1/1	0.79	0.16	69,69,69,69	0
56	MG	1A	3011	1/1	0.79	0.56	48,48,48,48	0
56	MG	2w	101	1/1	0.79	0.25	83,83,83,83	0
56	MG	2x	107	1/1	0.79	0.23	80,80,80,80	0
56	MG	2A	3501	1/1	0.80	0.13	74,74,74,74	0
56	MG	2A	3504	1/1	0.80	0.27	74,74,74,74	0
56	MG	1A	3485	1/1	0.80	0.14	64,64,64,64	0
56	MG	1A	3488	1/1	0.80	0.24	94,94,94,94	0
56	MG	2a	1722	1/1	0.80	0.14	79,79,79,79	0
56	MG	2A	3336	1/1	0.80	0.70	68,68,68,68	0
56	MG	1a	1773	1/1	0.80	0.12	59,59,59,59	0
56	MG	2A	3514	1/1	0.80	0.57	70,70,70,70	0
56	MG	1a	1897	1/1	0.80	0.12	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1a	1716	1/1	0.80	0.22	70,70,70,70	0
56	MG	2A	3344	1/1	0.80	0.22	47,47,47,47	0
56	MG	1A	3499	1/1	0.80	0.15	38,38,38,38	0
56	MG	1B	207	1/1	0.80	0.17	52,52,52,52	0
56	MG	1A	3313	1/1	0.80	0.14	75,75,75,75	0
56	MG	1A	3394	1/1	0.80	0.28	69,69,69,69	0
56	MG	2A	3542	1/1	0.80	0.16	83,83,83,83	0
56	MG	1x	104	1/1	0.80	0.37	76,76,76,76	0
56	MG	1x	111	1/1	0.80	0.16	70,70,70,70	0
56	MG	2a	1656	1/1	0.80	0.24	85,85,85,85	0
56	MG	2A	3464	1/1	0.80	0.20	82,82,82,82	0
56	MG	2A	3466	1/1	0.80	0.39	61,61,61,61	0
56	MG	2A	3378	1/1	0.80	0.58	57,57,57,57	0
56	MG	1a	1742	1/1	0.80	0.21	69,69,69,69	0
56	MG	1A	3449	1/1	0.80	0.30	51,51,51,51	0
56	MG	2A	3023	1/1	0.80	0.23	65,65,65,65	0
56	MG	1a	1881	1/1	0.80	0.51	70,70,70,70	0
56	MG	1A	3113	1/1	0.80	0.14	69,69,69,69	0
56	MG	2a	1695	1/1	0.80	0.07	80,80,80,80	0
56	MG	1a	1749	1/1	0.80	0.57	73,73,73,73	0
58	ZN	24	501	1/1	0.80	0.06	126,126,126,126	0
56	MG	1A	3533	1/1	0.81	0.26	44,44,44,44	0
56	MG	1A	3656	1/1	0.81	0.18	71,71,71,71	0
56	MG	2A	3132	1/1	0.81	0.20	84,84,84,84	0
56	MG	1A	3390	1/1	0.81	0.42	54,54,54,54	0
56	MG	2A	3454	1/1	0.81	0.41	81,81,81,81	0
56	MG	1A	3481	1/1	0.81	0.36	72,72,72,72	0
56	MG	2a	1731	1/1	0.81	0.23	72,72,72,72	0
56	MG	2a	1737	1/1	0.81	0.18	72,72,72,72	0
56	MG	1A	3880	1/1	0.81	0.32	66,66,66,66	0
56	MG	2a	1610	1/1	0.81	0.52	83,83,83,83	0
56	MG	2A	3162	1/1	0.81	0.13	59,59,59,59	0
56	MG	1A	3482	1/1	0.81	0.48	55,55,55,55	0
56	MG	1A	3883	1/1	0.81	0.45	43,43,43,43	0
56	MG	2A	3469	1/1	0.81	0.13	71,71,71,71	0
56	MG	2a	1781	1/1	0.81	0.24	73,73,73,73	0
56	MG	2a	1642	1/1	0.81	0.16	84,84,84,84	0
56	MG	2A	3237	1/1	0.81	0.15	55,55,55,55	0
56	MG	1A	3199	1/1	0.81	0.53	68,68,68,68	0
56	MG	2A	3555	1/1	0.81	0.18	58,58,58,58	0
56	MG	1A	3192	1/1	0.81	0.18	41,41,41,41	0
56	MG	2A	3289	1/1	0.81	0.08	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3452	1/1	0.81	0.17	52,52,52,52	0
56	MG	1A	3892	1/1	0.81	0.20	69,69,69,69	0
56	MG	2a	1811	1/1	0.81	0.10	79,79,79,79	0
56	MG	1A	3703	1/1	0.81	0.19	38,38,38,38	0
56	MG	2a	1817	1/1	0.81	0.11	75,75,75,75	0
56	MG	1E	301	1/1	0.81	0.13	37,37,37,37	0
56	MG	1a	1706	1/1	0.81	0.31	52,52,52,52	0
56	MG	2a	1826	1/1	0.81	0.14	59,59,59,59	0
56	MG	1O	3101	1/1	0.81	0.21	64,64,64,64	0
56	MG	1A	3642	1/1	0.81	0.20	63,63,63,63	0
56	MG	2A	3337	1/1	0.81	0.78	61,61,61,61	0
56	MG	1A	3507	1/1	0.81	0.22	49,49,49,49	0
56	MG	2F	302	1/1	0.81	0.10	69,69,69,69	0
56	MG	1a	1686	1/1	0.82	0.29	64,64,64,64	0
56	MG	2a	1694	1/1	0.82	0.08	77,77,77,77	0
56	MG	2A	3550	1/1	0.82	0.39	64,64,64,64	0
56	MG	1a	1880	1/1	0.82	0.11	81,81,81,81	0
56	MG	1A	3302	1/1	0.82	0.50	61,61,61,61	0
56	MG	1A	3599	1/1	0.82	0.13	57,57,57,57	0
56	MG	1A	3773	1/1	0.82	0.43	48,48,48,48	0
56	MG	16	101	1/1	0.82	0.26	52,52,52,52	0
56	MG	1A	3775	1/1	0.82	0.21	59,59,59,59	0
56	MG	1A	3193	1/1	0.82	0.28	55,55,55,55	0
56	MG	1a	1793	1/1	0.82	0.48	74,74,74,74	0
56	MG	2a	1729	1/1	0.82	0.14	84,84,84,84	0
56	MG	1B	218	1/1	0.82	0.17	76,76,76,76	0
56	MG	1A	3628	1/1	0.82	0.13	76,76,76,76	0
56	MG	1a	1905	1/1	0.82	0.10	73,73,73,73	0
56	MG	1a	1815	1/1	0.82	0.14	61,61,61,61	0
56	MG	1A	3647	1/1	0.82	0.10	91,91,91,91	0
56	MG	2a	1768	1/1	0.82	0.30	71,71,71,71	0
56	MG	2A	3102	1/1	0.82	0.38	66,66,66,66	0
56	MG	1A	3693	1/1	0.82	0.14	53,53,53,53	0
56	MG	1a	1838	1/1	0.82	0.57	74,74,74,74	0
56	MG	1a	1844	1/1	0.82	0.17	53,53,53,53	0
56	MG	1a	1929	1/1	0.82	0.41	87,87,87,87	0
56	MG	2A	3506	1/1	0.82	0.31	90,90,90,90	0
56	MG	1a	1616	1/1	0.82	0.23	61,61,61,61	0
56	MG	2a	1609	1/1	0.82	0.11	79,79,79,79	0
56	MG	1a	1853	1/1	0.82	0.33	81,81,81,81	0
56	MG	2A	3150	1/1	0.82	1.23	65,65,65,65	0
56	MG	2A	3154	1/1	0.82	0.52	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3515	1/1	0.82	0.60	86,86,86,86	0
56	MG	1A	3806	1/1	0.82	0.21	58,58,58,58	0
56	MG	2A	3160	1/1	0.82	0.33	57,57,57,57	0
56	MG	2A	3522	1/1	0.82	0.11	81,81,81,81	0
56	MG	1a	1662	1/1	0.82	0.30	76,76,76,76	0
56	MG	1a	1666	1/1	0.82	0.11	90,90,90,90	0
56	MG	2A	3418	1/1	0.82	0.14	70,70,70,70	0
56	MG	2A	3167	1/1	0.82	0.20	64,64,64,64	0
56	MG	1A	3833	1/1	0.82	0.16	67,67,67,67	0
56	MG	1A	3287	1/1	0.82	0.40	49,49,49,49	0
56	MG	1k	201	1/1	0.82	0.23	74,74,74,74	0
56	MG	2x	102	1/1	0.82	0.24	73,73,73,73	0
56	MG	1a	1876	1/1	0.82	0.42	83,83,83,83	0
56	MG	1A	3188	1/1	0.82	0.38	52,52,52,52	0
56	MG	1A	3758	1/1	0.83	0.13	58,58,58,58	0
56	MG	1a	1633	1/1	0.83	0.13	55,55,55,55	0
56	MG	1A	3884	1/1	0.83	0.64	59,59,59,59	0
56	MG	1A	3532	1/1	0.83	0.52	53,53,53,53	0
56	MG	2A	3465	1/1	0.83	0.18	76,76,76,76	0
56	MG	1A	3671	1/1	0.83	0.19	70,70,70,70	0
56	MG	2a	1707	1/1	0.83	0.12	72,72,72,72	0
56	MG	1A	3185	1/1	0.83	0.18	73,73,73,73	0
56	MG	1a	1676	1/1	0.83	0.42	73,73,73,73	0
56	MG	2A	3473	1/1	0.83	0.32	66,66,66,66	0
56	MG	1A	3399	1/1	0.83	0.31	51,51,51,51	0
56	MG	1A	3860	1/1	0.83	0.22	88,88,88,88	0
56	MG	2A	3492	1/1	0.83	0.18	69,69,69,69	0
56	MG	1A	3557	1/1	0.83	0.23	59,59,59,59	0
56	MG	1A	3611	1/1	0.83	0.24	57,57,57,57	0
56	MG	2F	304	1/1	0.83	0.16	75,75,75,75	0
56	MG	1a	1799	1/1	0.83	0.51	76,76,76,76	0
56	MG	2a	1754	1/1	0.83	0.37	63,63,63,63	0
56	MG	1A	3646	1/1	0.83	0.18	64,64,64,64	0
56	MG	1a	1814	1/1	0.83	0.19	76,76,76,76	0
56	MG	2A	3371	1/1	0.83	0.42	62,62,62,62	0
56	MG	1a	1709	1/1	0.83	0.26	68,68,68,68	0
56	MG	1a	1818	1/1	0.83	0.08	64,64,64,64	0
56	MG	13	104	1/1	0.83	0.12	70,70,70,70	0
56	MG	1A	3143	1/1	0.83	0.14	50,50,50,50	0
56	MG	2A	3512	1/1	0.83	0.17	85,85,85,85	0
56	MG	1A	3927	1/1	0.83	0.35	86,86,86,86	0
56	MG	2a	1798	1/1	0.83	0.50	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	1799	1/1	0.83	0.21	68,68,68,68	0
56	MG	1A	3928	1/1	0.83	0.50	62,62,62,62	0
56	MG	2a	1615	1/1	0.83	0.10	81,81,81,81	0
56	MG	1A	3235	1/1	0.83	0.31	55,55,55,55	0
56	MG	1A	3620	1/1	0.83	0.16	63,63,63,63	0
56	MG	2a	1624	1/1	0.83	0.32	61,61,61,61	0
56	MG	1B	201	1/1	0.83	0.16	63,63,63,63	0
56	MG	1a	1610	1/1	0.83	0.33	71,71,71,71	0
56	MG	2a	1816	1/1	0.83	0.14	89,89,89,89	0
56	MG	1a	1953	1/1	0.83	0.12	83,83,83,83	0
56	MG	1A	3393	1/1	0.83	0.34	53,53,53,53	0
56	MG	2A	3231	1/1	0.83	0.59	54,54,54,54	0
56	MG	1a	1858	1/1	0.83	0.10	68,68,68,68	0
56	MG	1l	203	1/1	0.83	0.16	71,71,71,71	0
56	MG	2v	101	1/1	0.83	0.20	61,61,61,61	0
56	MG	1a	1612	1/1	0.83	0.34	72,72,72,72	0
56	MG	1a	1867	1/1	0.83	0.08	72,72,72,72	0
56	MG	1A	3508	1/1	0.83	0.24	63,63,63,63	0
56	MG	1a	1755	1/1	0.83	0.35	68,68,68,68	0
56	MG	1A	3636	1/1	0.83	0.12	62,62,62,62	0
56	MG	2A	3411	1/1	0.84	0.54	69,69,69,69	0
56	MG	1A	3438	1/1	0.84	0.20	78,78,78,78	0
56	MG	2a	1680	1/1	0.84	0.16	67,67,67,67	0
56	MG	1A	3750	1/1	0.84	0.27	67,67,67,67	0
56	MG	2A	3538	1/1	0.84	0.09	66,66,66,66	0
56	MG	1A	3400	1/1	0.84	0.49	66,66,66,66	0
56	MG	2A	3426	1/1	0.84	0.21	56,56,56,56	0
56	MG	18	103	1/1	0.84	0.18	58,58,58,58	0
56	MG	1A	3542	1/1	0.84	0.21	40,40,40,40	0
56	MG	2A	3440	1/1	0.84	0.23	57,57,57,57	0
56	MG	1A	3024	1/1	0.84	0.16	74,74,74,74	0
56	MG	2A	3552	1/1	0.84	0.15	70,70,70,70	0
56	MG	1a	1606	1/1	0.84	0.22	74,74,74,74	0
56	MG	1a	1607	1/1	0.84	0.50	63,63,63,63	0
56	MG	1a	1608	1/1	0.84	0.36	65,65,65,65	0
56	MG	2A	3561	1/1	0.84	0.17	64,64,64,64	0
56	MG	1a	1740	1/1	0.84	0.18	67,67,67,67	0
56	MG	2A	3564	1/1	0.84	0.35	65,65,65,65	0
56	MG	1A	3397	1/1	0.84	0.19	60,60,60,60	0
56	MG	1A	3849	1/1	0.84	0.15	68,68,68,68	0
56	MG	1a	1862	1/1	0.84	0.18	78,78,78,78	0
56	MG	1B	208	1/1	0.84	0.22	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1o	101	1/1	0.84	0.17	80,80,80,80	0
56	MG	1A	3398	1/1	0.84	0.18	78,78,78,78	0
56	MG	1a	1871	1/1	0.84	0.28	53,53,53,53	0
56	MG	1A	3616	1/1	0.84	0.58	48,48,48,48	0
56	MG	1a	1758	1/1	0.84	0.19	65,65,65,65	0
56	MG	1A	3512	1/1	0.84	0.25	39,39,39,39	0
56	MG	2A	3476	1/1	0.84	0.18	69,69,69,69	0
56	MG	2Q	201	1/1	0.84	0.19	71,71,71,71	0
56	MG	1x	102	1/1	0.84	0.81	80,80,80,80	0
56	MG	1A	3598	1/1	0.84	0.48	60,60,60,60	0
56	MG	1a	1626	1/1	0.84	0.10	75,75,75,75	0
56	MG	1A	3627	1/1	0.84	0.18	56,56,56,56	0
56	MG	1A	3785	1/1	0.84	0.41	73,73,73,73	0
56	MG	2A	3016	1/1	0.84	0.19	58,58,58,58	0
56	MG	1D	303	1/1	0.84	0.38	65,65,65,65	0
56	MG	1A	3863	1/1	0.84	0.11	60,60,60,60	0
56	MG	1F	301	1/1	0.84	0.22	52,52,52,52	0
56	MG	1a	1891	1/1	0.84	0.23	78,78,78,78	0
56	MG	2A	3366	1/1	0.84	0.21	66,66,66,66	0
56	MG	1A	3918	1/1	0.84	0.26	55,55,55,55	0
56	MG	1a	1896	1/1	0.84	0.13	73,73,73,73	0
56	MG	2a	1821	1/1	0.84	0.63	67,67,67,67	0
56	MG	2A	3063	1/1	0.84	0.27	69,69,69,69	0
56	MG	1a	1679	1/1	0.84	0.22	70,70,70,70	0
56	MG	1A	3164	1/1	0.84	0.40	38,38,38,38	0
56	MG	2a	1649	1/1	0.84	0.12	81,81,81,81	0
56	MG	1a	1683	1/1	0.84	0.26	75,75,75,75	0
56	MG	1V	202	1/1	0.84	0.19	47,47,47,47	0
56	MG	1a	1908	1/1	0.84	0.33	72,72,72,72	0
56	MG	1A	3629	1/1	0.84	0.34	73,73,73,73	0
56	MG	1A	3798	1/1	0.84	0.23	64,64,64,64	0
56	MG	2A	3135	1/1	0.84	0.26	68,68,68,68	0
56	MG	1A	3254	1/1	0.85	0.21	45,45,45,45	0
56	MG	1A	3766	1/1	0.85	0.16	98,98,98,98	0
56	MG	1A	3217	1/1	0.85	0.25	63,63,63,63	0
56	MG	2A	3370	1/1	0.85	0.22	60,60,60,60	0
56	MG	1A	3404	1/1	0.85	0.13	58,58,58,58	0
56	MG	1A	3893	1/1	0.85	0.20	41,41,41,41	0
56	MG	2A	3091	1/1	0.85	0.23	59,59,59,59	0
56	MG	1A	3016	1/1	0.85	0.22	61,61,61,61	0
56	MG	2A	3386	1/1	0.85	0.14	66,66,66,66	0
56	MG	1A	3058	1/1	0.85	0.12	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3910	1/1	0.85	0.18	54,54,54,54	0
56	MG	1A	3914	1/1	0.85	0.15	64,64,64,64	0
56	MG	1A	3781	1/1	0.85	0.16	60,60,60,60	0
56	MG	1A	3917	1/1	0.85	0.46	67,67,67,67	0
56	MG	1A	3180	1/1	0.85	0.12	56,56,56,56	0
56	MG	2A	3140	1/1	0.85	0.25	71,71,71,71	0
56	MG	1A	3134	1/1	0.85	0.28	64,64,64,64	0
56	MG	2A	3417	1/1	0.85	0.12	68,68,68,68	0
56	MG	1A	3567	1/1	0.85	0.46	37,37,37,37	0
56	MG	1a	1941	1/1	0.85	0.14	55,55,55,55	0
56	MG	2A	3554	1/1	0.85	0.11	74,74,74,74	0
56	MG	2A	3158	1/1	0.85	0.18	66,66,66,66	0
56	MG	1A	3926	1/1	0.85	0.33	83,83,83,83	0
56	MG	1A	3864	1/1	0.85	0.38	68,68,68,68	0
56	MG	1a	1726	1/1	0.85	0.30	75,75,75,75	0
56	MG	1A	3586	1/1	0.85	0.35	54,54,54,54	0
56	MG	1a	1605	1/1	0.85	0.49	63,63,63,63	0
56	MG	2a	1750	1/1	0.85	0.27	61,61,61,61	0
56	MG	2A	3169	1/1	0.85	0.15	67,67,67,67	0
56	MG	2a	1760	1/1	0.85	0.25	61,61,61,61	0
56	MG	2a	1764	1/1	0.85	0.23	75,75,75,75	0
56	MG	1d	302	1/1	0.85	0.10	81,81,81,81	0
56	MG	1A	3136	1/1	0.85	0.27	56,56,56,56	0
56	MG	1i	201	1/1	0.85	0.37	84,84,84,84	0
56	MG	1A	3867	1/1	0.85	0.46	53,53,53,53	0
56	MG	2A	3261	1/1	0.85	0.31	71,71,71,71	0
56	MG	1A	3932	1/1	0.85	0.37	65,65,65,65	0
56	MG	1A	3800	1/1	0.85	0.10	68,68,68,68	0
56	MG	2a	1783	1/1	0.85	0.14	60,60,60,60	0
56	MG	1a	1868	1/1	0.85	0.21	68,68,68,68	0
56	MG	2a	1786	1/1	0.85	0.17	72,72,72,72	0
56	MG	1A	3076	1/1	0.85	0.21	45,45,45,45	0
56	MG	2A	3294	1/1	0.85	1.15	64,64,64,64	0
56	MG	2A	3470	1/1	0.85	0.12	68,68,68,68	0
56	MG	2A	3295	1/1	0.85	0.36	57,57,57,57	0
56	MG	2A	3472	1/1	0.85	0.31	84,84,84,84	0
56	MG	2A	3300	1/1	0.85	0.34	53,53,53,53	0
56	MG	1B	204	1/1	0.85	0.15	63,63,63,63	0
56	MG	1A	3006	1/1	0.85	0.36	59,59,59,59	0
56	MG	2a	1603	1/1	0.85	0.51	67,67,67,67	0
56	MG	1A	3809	1/1	0.85	0.44	86,86,86,86	0
56	MG	1a	1760	1/1	0.85	0.59	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3493	1/1	0.85	0.16	76,76,76,76	0
56	MG	1A	3817	1/1	0.85	0.23	49,49,49,49	0
56	MG	1a	1768	1/1	0.85	0.71	75,75,75,75	0
56	MG	2a	1823	1/1	0.85	0.20	88,88,88,88	0
56	MG	1x	120	1/1	0.85	0.43	80,80,80,80	0
56	MG	1B	209	1/1	0.85	0.32	67,67,67,67	0
56	MG	1a	1623	1/1	0.85	0.32	66,66,66,66	0
56	MG	1A	3667	1/1	0.85	0.32	71,71,71,71	0
56	MG	1a	1627	1/1	0.85	0.10	70,70,70,70	0
56	MG	2A	3350	1/1	0.85	0.26	66,66,66,66	0
56	MG	2a	1646	1/1	0.85	0.35	58,58,58,58	0
56	MG	1A	3835	1/1	0.85	0.16	59,59,59,59	0
56	MG	1A	3378	1/1	0.85	0.63	56,56,56,56	0
56	MG	1A	3170	1/1	0.86	0.60	73,73,73,73	0
56	MG	2A	3556	1/1	0.86	0.23	56,56,56,56	0
56	MG	2A	3460	1/1	0.86	0.15	46,46,46,46	0
56	MG	2A	3086	1/1	0.86	0.20	67,67,67,67	0
56	MG	1a	1938	1/1	0.86	0.27	84,84,84,84	0
56	MG	1A	3161	1/1	0.86	0.33	67,67,67,67	0
56	MG	1A	3755	1/1	0.86	0.09	54,54,54,54	0
56	MG	1A	3455	1/1	0.86	0.43	41,41,41,41	0
56	MG	2a	1715	1/1	0.86	0.18	69,69,69,69	0
56	MG	1A	3145	1/1	0.86	0.18	52,52,52,52	0
56	MG	1a	1688	1/1	0.86	0.61	72,72,72,72	0
56	MG	1A	3230	1/1	0.86	0.26	76,76,76,76	0
56	MG	2A	3355	1/1	0.86	0.19	76,76,76,76	0
56	MG	2A	3356	1/1	0.86	0.25	54,54,54,54	0
56	MG	1A	3207	1/1	0.86	0.37	59,59,59,59	0
56	MG	2a	1732	1/1	0.86	0.21	90,90,90,90	0
56	MG	1a	1780	1/1	0.86	0.12	67,67,67,67	0
56	MG	1a	1698	1/1	0.86	0.10	75,75,75,75	0
56	MG	1A	3158	1/1	0.86	0.70	41,41,41,41	0
56	MG	2a	1747	1/1	0.86	0.22	72,72,72,72	0
56	MG	1l	202	1/1	0.86	0.79	70,70,70,70	0
56	MG	1a	1787	1/1	0.86	0.10	83,83,83,83	0
56	MG	2A	3375	1/1	0.86	0.30	56,56,56,56	0
56	MG	2A	3499	1/1	0.86	0.55	73,73,73,73	0
56	MG	1A	3672	1/1	0.86	0.16	48,48,48,48	0
56	MG	1A	3303	1/1	0.86	0.10	42,42,42,42	0
56	MG	1A	3494	1/1	0.86	0.32	69,69,69,69	0
56	MG	1v	101	1/1	0.86	0.15	73,73,73,73	0
56	MG	2a	1604	1/1	0.86	0.44	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3858	1/1	0.86	0.16	71,71,71,71	0
56	MG	1A	3312	1/1	0.86	0.27	65,65,65,65	0
56	MG	2A	3171	1/1	0.86	0.56	51,51,51,51	0
56	MG	1A	3504	1/1	0.86	0.23	37,37,37,37	0
56	MG	1A	3704	1/1	0.86	0.12	49,49,49,49	0
56	MG	2a	1792	1/1	0.86	0.29	59,59,59,59	0
56	MG	2a	1795	1/1	0.86	0.06	85,85,85,85	0
56	MG	1A	3250	1/1	0.86	0.22	59,59,59,59	0
56	MG	2A	3244	1/1	0.86	0.59	59,59,59,59	0
56	MG	1A	3708	1/1	0.86	0.15	33,33,33,33	0
56	MG	1x	119	1/1	0.86	0.24	78,78,78,78	0
56	MG	2a	1631	1/1	0.86	0.09	100,100,100,100	0
56	MG	1A	3711	1/1	0.86	0.09	46,46,46,46	0
56	MG	1a	1907	1/1	0.86	0.17	68,68,68,68	0
56	MG	1F	303	1/1	0.86	0.20	75,75,75,75	0
56	MG	1A	3428	1/1	0.86	0.53	69,69,69,69	0
56	MG	2a	1650	1/1	0.86	0.14	73,73,73,73	0
56	MG	1A	3169	1/1	0.86	0.45	48,48,48,48	0
56	MG	2A	3439	1/1	0.86	0.16	75,75,75,75	0
56	MG	2a	1820	1/1	0.86	0.19	58,58,58,58	0
56	MG	2a	1661	1/1	0.86	0.17	79,79,79,79	0
56	MG	1A	3336	1/1	0.86	0.14	54,54,54,54	0
56	MG	1a	1754	1/1	0.86	0.16	62,62,62,62	0
56	MG	2A	3325	1/1	0.86	0.25	62,62,62,62	0
56	MG	1W	202	1/1	0.86	0.42	47,47,47,47	0
56	MG	2a	1670	1/1	0.86	0.14	74,74,74,74	0
56	MG	2A	3328	1/1	0.86	0.29	69,69,69,69	0
56	MG	1a	1926	1/1	0.86	0.18	77,77,77,77	0
56	MG	1A	3874	1/1	0.86	0.12	65,65,65,65	0
56	MG	1A	3343	1/1	0.86	0.24	44,44,44,44	0
56	MG	2A	3458	1/1	0.86	0.18	73,73,73,73	0
56	MG	2a	1691	1/1	0.86	0.24	90,90,90,90	0
56	MG	2a	1703	1/1	0.87	0.19	67,67,67,67	0
56	MG	1A	3645	1/1	0.87	0.32	60,60,60,60	0
56	MG	1a	1804	1/1	0.87	0.51	57,57,57,57	0
56	MG	1a	1913	1/1	0.87	0.19	66,66,66,66	0
56	MG	1A	3877	1/1	0.87	0.34	70,70,70,70	0
56	MG	1A	3741	1/1	0.87	0.17	49,49,49,49	0
56	MG	1A	3189	1/1	0.87	0.34	51,51,51,51	0
56	MG	2a	1724	1/1	0.87	0.12	77,77,77,77	0
56	MG	1a	1717	1/1	0.87	0.20	77,77,77,77	0
56	MG	2A	3346	1/1	0.87	0.23	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3231	1/1	0.87	0.23	51,51,51,51	0
56	MG	1A	3141	1/1	0.87	0.12	75,75,75,75	0
56	MG	1a	1931	1/1	0.87	0.09	92,92,92,92	0
56	MG	2A	3489	1/1	0.87	0.12	72,72,72,72	0
56	MG	2A	3490	1/1	0.87	0.26	68,68,68,68	0
56	MG	1A	3019	1/1	0.87	0.24	63,63,63,63	0
56	MG	1a	1736	1/1	0.87	0.45	79,79,79,79	0
56	MG	1a	1850	1/1	0.87	0.15	73,73,73,73	0
56	MG	1B	216	1/1	0.87	0.42	67,67,67,67	0
56	MG	2a	1758	1/1	0.87	0.32	61,61,61,61	0
56	MG	1A	3752	1/1	0.87	0.08	71,71,71,71	0
56	MG	1A	3657	1/1	0.87	0.15	69,69,69,69	0
56	MG	2a	1767	1/1	0.87	0.50	59,59,59,59	0
56	MG	1A	3442	1/1	0.87	0.30	54,54,54,54	0
56	MG	1A	3210	1/1	0.87	0.79	47,47,47,47	0
56	MG	1A	3851	1/1	0.87	0.33	61,61,61,61	0
56	MG	1A	3184	1/1	0.87	0.15	61,61,61,61	0
56	MG	1A	3318	1/1	0.87	0.31	64,64,64,64	0
56	MG	1A	3155	1/1	0.87	0.24	59,59,59,59	0
56	MG	1a	1869	1/1	0.87	0.12	64,64,64,64	0
56	MG	1a	1628	1/1	0.87	0.21	55,55,55,55	0
56	MG	1A	3471	1/1	0.87	0.25	66,66,66,66	0
56	MG	1a	1657	1/1	0.87	0.18	46,46,46,46	0
56	MG	2A	3190	1/1	0.87	0.22	61,61,61,61	0
56	MG	2A	3197	1/1	0.87	0.37	66,66,66,66	0
56	MG	2A	3220	1/1	0.87	0.56	59,59,59,59	0
56	MG	1A	3859	1/1	0.87	0.21	69,69,69,69	0
56	MG	1G	202	1/1	0.87	0.11	47,47,47,47	0
56	MG	1A	3480	1/1	0.87	0.18	74,74,74,74	0
56	MG	1A	3067	1/1	0.87	0.17	75,75,75,75	0
56	MG	1A	3564	1/1	0.87	0.69	43,43,43,43	0
56	MG	1W	201	1/1	0.87	0.29	57,57,57,57	0
56	MG	1a	1885	1/1	0.87	0.16	71,71,71,71	0
56	MG	1A	3633	1/1	0.87	0.12	70,70,70,70	0
56	MG	1A	3396	1/1	0.87	0.28	61,61,61,61	0
56	MG	1A	3576	1/1	0.87	0.22	22,22,22,22	0
56	MG	1A	3174	1/1	0.87	0.38	63,63,63,63	0
56	MG	2a	1818	1/1	0.87	0.15	86,86,86,86	0
56	MG	2A	3445	1/1	0.87	0.13	84,84,84,84	0
56	MG	2A	3549	1/1	0.87	0.21	53,53,53,53	0
56	MG	1a	1786	1/1	0.87	0.15	75,75,75,75	0
56	MG	1A	3424	1/1	0.87	0.20	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3305	1/1	0.87	0.19	60,60,60,60	0
56	MG	2a	1687	1/1	0.87	0.11	71,71,71,71	0
56	MG	2a	1688	1/1	0.87	0.10	72,72,72,72	0
56	MG	1a	1692	1/1	0.87	0.10	86,86,86,86	0
56	MG	2A	3017	1/1	0.87	0.23	53,53,53,53	0
56	MG	18	101	1/1	0.87	0.44	53,53,53,53	0
56	MG	1A	3427	1/1	0.87	0.19	43,43,43,43	0
56	MG	1A	3496	1/1	0.87	0.21	47,47,47,47	0
56	MG	2A	3032	1/1	0.87	0.15	68,68,68,68	0
56	MG	1a	1604	1/1	0.88	0.46	62,62,62,62	0
56	MG	1A	3765	1/1	0.88	0.56	60,60,60,60	0
56	MG	1A	3412	1/1	0.88	0.16	49,49,49,49	0
56	MG	1A	3769	1/1	0.88	0.10	66,66,66,66	0
56	MG	1x	107	1/1	0.88	0.10	71,71,71,71	0
56	MG	1x	109	1/1	0.88	0.21	56,56,56,56	0
56	MG	1A	3624	1/1	0.88	0.30	40,40,40,40	0
56	MG	1x	115	1/1	0.88	0.27	79,79,79,79	0
56	MG	1a	1744	1/1	0.88	0.42	64,64,64,64	0
56	MG	1A	3413	1/1	0.88	0.77	43,43,43,43	0
56	MG	1A	3476	1/1	0.88	0.34	63,63,63,63	0
56	MG	1a	1747	1/1	0.88	0.31	63,63,63,63	0
56	MG	1A	3163	1/1	0.88	0.38	67,67,67,67	0
56	MG	1A	3420	1/1	0.88	0.15	32,32,32,32	0
56	MG	2A	3018	1/1	0.88	0.23	32,32,32,32	0
56	MG	2A	3348	1/1	0.88	0.36	50,50,50,50	0
56	MG	2A	3020	1/1	0.88	0.18	72,72,72,72	0
56	MG	1A	3700	1/1	0.88	0.23	72,72,72,72	0
56	MG	1A	3327	1/1	0.88	0.20	62,62,62,62	0
56	MG	1A	3790	1/1	0.88	0.50	66,66,66,66	0
56	MG	1a	1761	1/1	0.88	0.48	69,69,69,69	0
56	MG	1A	3049	1/1	0.88	0.12	38,38,38,38	0
56	MG	1a	1625	1/1	0.88	0.15	72,72,72,72	0
56	MG	1B	217	1/1	0.88	0.24	64,64,64,64	0
56	MG	2A	3369	1/1	0.88	0.36	68,68,68,68	0
56	MG	1A	3263	1/1	0.88	0.28	31,31,31,31	0
56	MG	2A	3539	1/1	0.88	0.11	86,86,86,86	0
56	MG	1A	3587	1/1	0.88	0.33	40,40,40,40	0
56	MG	1a	1632	1/1	0.88	0.11	54,54,54,54	0
56	MG	1B	221	1/1	0.88	0.41	58,58,58,58	0
56	MG	2a	1726	1/1	0.88	0.20	65,65,65,65	0
56	MG	1a	1647	1/1	0.88	0.14	54,54,54,54	0
56	MG	2A	3108	1/1	0.88	0.47	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3548	1/1	0.88	0.19	58,58,58,58	0
56	MG	1a	1653	1/1	0.88	0.24	60,60,60,60	0
56	MG	2A	3123	1/1	0.88	0.33	33,33,33,33	0
56	MG	1A	3590	1/1	0.88	0.42	55,55,55,55	0
56	MG	1A	3492	1/1	0.88	0.17	44,44,44,44	0
56	MG	1A	3805	1/1	0.88	0.27	74,74,74,74	0
56	MG	2a	1749	1/1	0.88	0.19	62,62,62,62	0
56	MG	1A	3081	1/1	0.88	0.18	51,51,51,51	0
56	MG	1a	1922	1/1	0.88	0.18	82,82,82,82	0
56	MG	1A	3727	1/1	0.88	0.19	65,65,65,65	0
56	MG	2A	3143	1/1	0.88	0.23	59,59,59,59	0
56	MG	1A	3885	1/1	0.88	0.51	53,53,53,53	0
56	MG	1A	3811	1/1	0.88	0.09	81,81,81,81	0
56	MG	1A	3812	1/1	0.88	0.17	68,68,68,68	0
56	MG	1A	3728	1/1	0.88	0.22	48,48,48,48	0
56	MG	1a	1932	1/1	0.88	0.14	72,72,72,72	0
56	MG	2a	1774	1/1	0.88	0.17	79,79,79,79	0
56	MG	2A	3431	1/1	0.88	0.10	70,70,70,70	0
56	MG	1A	3822	1/1	0.88	0.14	57,57,57,57	0
56	MG	1a	1808	1/1	0.88	0.16	60,60,60,60	0
56	MG	1A	3152	1/1	0.88	0.28	55,55,55,55	0
56	MG	2D	302	1/1	0.88	0.28	68,68,68,68	0
56	MG	1A	3212	1/1	0.88	0.23	52,52,52,52	0
56	MG	1A	3905	1/1	0.88	0.12	70,70,70,70	0
56	MG	1a	1944	1/1	0.88	0.09	70,70,70,70	0
56	MG	2a	1794	1/1	0.88	0.08	88,88,88,88	0
56	MG	1A	3377	1/1	0.88	0.37	63,63,63,63	0
56	MG	2A	3192	1/1	0.88	0.51	36,36,36,36	0
56	MG	1A	3648	1/1	0.88	0.14	77,77,77,77	0
56	MG	2A	3213	1/1	0.88	0.34	48,48,48,48	0
56	MG	2A	3455	1/1	0.88	0.51	56,56,56,56	0
56	MG	2A	3218	1/1	0.88	0.42	56,56,56,56	0
56	MG	12	101	1/1	0.88	0.48	73,73,73,73	0
56	MG	1a	1841	1/1	0.88	0.09	72,72,72,72	0
56	MG	1d	301	1/1	0.88	0.17	62,62,62,62	0
56	MG	1A	3842	1/1	0.88	0.27	63,63,63,63	0
56	MG	2a	1606	1/1	0.88	0.61	87,87,87,87	0
56	MG	2a	1815	1/1	0.88	0.24	71,71,71,71	0
56	MG	1a	1711	1/1	0.88	0.47	75,75,75,75	0
56	MG	2A	3245	1/1	0.88	0.26	63,63,63,63	0
56	MG	1A	3240	1/1	0.88	0.44	49,49,49,49	0
56	MG	1A	3655	1/1	0.88	0.10	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3263	1/1	0.88	0.32	48,48,48,48	0
56	MG	2a	1618	1/1	0.88	0.18	129,129,129,129	0
56	MG	2A	3268	1/1	0.88	0.12	77,77,77,77	0
56	MG	1A	3441	1/1	0.88	0.21	26,26,26,26	0
56	MG	1A	3153	1/1	0.88	0.15	65,65,65,65	0
56	MG	1a	1723	1/1	0.88	0.15	80,80,80,80	0
56	MG	2q	201	1/1	0.88	0.12	72,72,72,72	0
56	MG	2a	1636	1/1	0.88	0.18	69,69,69,69	0
56	MG	2A	3480	1/1	0.88	0.44	70,70,70,70	0
56	MG	1A	3385	1/1	0.88	0.52	59,59,59,59	0
56	MG	1a	1859	1/1	0.88	0.10	79,79,79,79	0
56	MG	2x	103	1/1	0.88	0.17	83,83,83,83	0
56	MG	1A	3178	1/1	0.88	0.36	57,57,57,57	0
56	MG	1A	3219	1/1	0.88	0.37	55,55,55,55	0
56	MG	2a	1677	1/1	0.89	0.09	67,67,67,67	0
56	MG	1w	102	1/1	0.89	0.22	63,63,63,63	0
56	MG	2A	3525	1/1	0.89	0.54	81,81,81,81	0
56	MG	2A	3396	1/1	0.89	0.54	63,63,63,63	0
56	MG	1A	3053	1/1	0.89	0.21	40,40,40,40	0
56	MG	1A	3919	1/1	0.89	0.44	85,85,85,85	0
56	MG	1w	105	1/1	0.89	0.35	55,55,55,55	0
56	MG	2A	3536	1/1	0.89	0.37	57,57,57,57	0
56	MG	1A	3194	1/1	0.89	0.27	58,58,58,58	0
56	MG	2A	3413	1/1	0.89	0.29	47,47,47,47	0
56	MG	1a	1682	1/1	0.89	0.10	62,62,62,62	0
56	MG	1a	1781	1/1	0.89	0.12	75,75,75,75	0
56	MG	1A	3159	1/1	0.89	0.20	54,54,54,54	0
56	MG	1a	1783	1/1	0.89	0.27	47,47,47,47	0
56	MG	2a	1701	1/1	0.89	0.11	61,61,61,61	0
56	MG	2A	3243	1/1	0.89	0.67	53,53,53,53	0
56	MG	1A	3226	1/1	0.89	0.14	61,61,61,61	0
56	MG	1A	3794	1/1	0.89	0.19	59,59,59,59	0
56	MG	1A	3079	1/1	0.89	0.32	54,54,54,54	0
56	MG	2A	3436	1/1	0.89	0.30	61,61,61,61	0
56	MG	2a	1719	1/1	0.89	0.29	70,70,70,70	0
56	MG	1a	1789	1/1	0.89	0.07	77,77,77,77	0
56	MG	1x	124	1/1	0.89	0.20	65,65,65,65	0
56	MG	1A	3338	1/1	0.89	0.16	52,52,52,52	0
56	MG	2A	3007	1/1	0.89	0.09	72,72,72,72	0
56	MG	1A	3103	1/1	0.89	0.44	62,62,62,62	0
56	MG	2A	3446	1/1	0.89	0.27	60,60,60,60	0
56	MG	1A	3501	1/1	0.89	0.12	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3870	1/1	0.89	0.22	61,61,61,61	0
56	MG	1A	3353	1/1	0.89	0.38	27,27,27,27	0
56	MG	1A	3172	1/1	0.89	0.10	79,79,79,79	0
56	MG	1A	3298	1/1	0.89	0.14	58,58,58,58	0
56	MG	2B	204	1/1	0.89	0.35	60,60,60,60	0
56	MG	2A	3303	1/1	0.89	0.74	56,56,56,56	0
56	MG	2A	3304	1/1	0.89	0.21	56,56,56,56	0
56	MG	1a	1920	1/1	0.89	0.07	66,66,66,66	0
56	MG	2A	3315	1/1	0.89	0.32	57,57,57,57	0
56	MG	1A	3014	1/1	0.89	0.25	59,59,59,59	0
56	MG	2E	302	1/1	0.89	0.27	36,36,36,36	0
56	MG	1A	3815	1/1	0.89	0.17	45,45,45,45	0
56	MG	1A	3754	1/1	0.89	0.11	52,52,52,52	0
56	MG	2A	3057	1/1	0.89	0.27	52,52,52,52	0
56	MG	1A	3082	1/1	0.89	0.24	67,67,67,67	0
56	MG	1A	3832	1/1	0.89	0.24	53,53,53,53	0
56	MG	1a	1835	1/1	0.89	0.08	83,83,83,83	0
56	MG	1A	3379	1/1	0.89	0.22	56,56,56,56	0
56	MG	1B	219	1/1	0.89	0.23	59,59,59,59	0
56	MG	2A	3474	1/1	0.89	0.34	67,67,67,67	0
56	MG	1A	3457	1/1	0.89	0.34	46,46,46,46	0
56	MG	1A	3460	1/1	0.89	0.15	53,53,53,53	0
56	MG	1A	3554	1/1	0.89	0.25	54,54,54,54	0
56	MG	1B	225	1/1	0.89	0.07	80,80,80,80	0
56	MG	1a	1741	1/1	0.89	0.17	73,73,73,73	0
56	MG	2a	1793	1/1	0.89	0.08	73,73,73,73	0
56	MG	2A	3129	1/1	0.89	0.19	73,73,73,73	0
56	MG	2A	3491	1/1	0.89	0.17	68,68,68,68	0
56	MG	1a	1620	1/1	0.89	0.13	72,72,72,72	0
56	MG	1A	3461	1/1	0.89	0.72	58,58,58,58	0
56	MG	2A	3494	1/1	0.89	0.09	79,79,79,79	0
56	MG	2a	1617	1/1	0.89	0.09	101,101,101,101	0
56	MG	1A	3843	1/1	0.89	0.07	69,69,69,69	0
56	MG	2a	1619	1/1	0.89	0.08	80,80,80,80	0
56	MG	2a	1620	1/1	0.89	0.16	92,92,92,92	0
56	MG	2a	1806	1/1	0.89	0.10	90,90,90,90	0
56	MG	1A	3689	1/1	0.89	0.23	55,55,55,55	0
56	MG	1A	3411	1/1	0.89	0.20	54,54,54,54	0
56	MG	1A	3191	1/1	0.89	0.18	57,57,57,57	0
56	MG	2A	3363	1/1	0.89	0.13	65,65,65,65	0
56	MG	1E	304	1/1	0.89	0.22	70,70,70,70	0
56	MG	2a	1637	1/1	0.89	0.25	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3306	1/1	0.89	0.33	50,50,50,50	0
56	MG	1A	3478	1/1	0.89	0.16	60,60,60,60	0
56	MG	1G	201	1/1	0.89	0.12	38,38,38,38	0
56	MG	1A	3308	1/1	0.89	0.28	46,46,46,46	0
56	MG	2A	3373	1/1	0.89	0.13	69,69,69,69	0
56	MG	1a	1661	1/1	0.89	0.37	57,57,57,57	0
56	MG	1A	3783	1/1	0.89	0.28	56,56,56,56	0
56	MG	1A	3012	1/1	0.89	0.56	51,51,51,51	0
56	MG	1T	201	1/1	0.89	0.26	55,55,55,55	0
56	MG	1v	102	1/1	0.89	0.17	67,67,67,67	0
56	MG	1U	202	1/1	0.89	0.20	43,43,43,43	0
56	MG	2A	3175	1/1	0.89	0.20	52,52,52,52	0
56	MG	2a	1669	1/1	0.89	0.09	91,91,91,91	0
56	MG	2A	3523	1/1	0.89	0.18	63,63,63,63	0
56	MG	2a	1671	1/1	0.89	0.24	88,88,88,88	0
56	MG	2a	1672	1/1	0.89	0.08	94,94,94,94	0
56	MG	2a	1634	1/1	0.90	0.12	59,59,59,59	0
56	MG	1A	3429	1/1	0.90	0.28	59,59,59,59	0
56	MG	1A	3771	1/1	0.90	0.16	64,64,64,64	0
56	MG	2a	1639	1/1	0.90	0.11	71,71,71,71	0
56	MG	1A	3296	1/1	0.90	0.28	73,73,73,73	0
56	MG	1A	3433	1/1	0.90	0.21	41,41,41,41	0
56	MG	1B	206	1/1	0.90	0.10	61,61,61,61	0
56	MG	2a	1647	1/1	0.90	0.22	54,54,54,54	0
56	MG	2a	1648	1/1	0.90	0.23	76,76,76,76	0
56	MG	1A	3087	1/1	0.90	0.83	40,40,40,40	0
56	MG	1A	3670	1/1	0.90	0.19	53,53,53,53	0
56	MG	2A	3301	1/1	0.90	0.09	65,65,65,65	0
56	MG	2A	3302	1/1	0.90	0.24	41,41,41,41	0
56	MG	2a	1658	1/1	0.90	0.12	77,77,77,77	0
56	MG	1a	1619	1/1	0.90	0.16	71,71,71,71	0
56	MG	1A	3500	1/1	0.90	0.14	61,61,61,61	0
56	MG	1a	1887	1/1	0.90	0.09	75,75,75,75	0
56	MG	2A	3008	1/1	0.90	0.17	57,57,57,57	0
56	MG	2a	1666	1/1	0.90	0.15	75,75,75,75	0
56	MG	2A	3011	1/1	0.90	0.25	55,55,55,55	0
56	MG	2A	3497	1/1	0.90	0.19	71,71,71,71	0
56	MG	1B	212	1/1	0.90	0.26	62,62,62,62	0
56	MG	1A	3215	1/1	0.90	0.35	67,67,67,67	0
56	MG	1a	1762	1/1	0.90	0.36	70,70,70,70	0
56	MG	1A	3613	1/1	0.90	0.11	52,52,52,52	0
56	MG	2A	3503	1/1	0.90	0.41	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1a	1764	1/1	0.90	0.06	69,69,69,69	0
56	MG	1A	3787	1/1	0.90	0.24	57,57,57,57	0
56	MG	2a	1684	1/1	0.90	0.09	74,74,74,74	0
56	MG	1A	3789	1/1	0.90	0.09	78,78,78,78	0
56	MG	2A	3508	1/1	0.90	0.14	68,68,68,68	0
56	MG	1A	3018	1/1	0.90	0.51	66,66,66,66	0
56	MG	2A	3036	1/1	0.90	0.13	68,68,68,68	0
56	MG	1A	3791	1/1	0.90	0.40	54,54,54,54	0
56	MG	2a	1693	1/1	0.90	0.11	85,85,85,85	0
56	MG	1a	1638	1/1	0.90	0.33	58,58,58,58	0
56	MG	2A	3054	1/1	0.90	0.23	57,57,57,57	0
56	MG	2a	1697	1/1	0.90	0.19	69,69,69,69	0
56	MG	1A	3374	1/1	0.90	0.15	57,57,57,57	0
56	MG	1a	1651	1/1	0.90	0.37	56,56,56,56	0
56	MG	1A	3128	1/1	0.90	0.16	62,62,62,62	0
56	MG	2A	3066	1/1	0.90	0.21	59,59,59,59	0
56	MG	1A	3510	1/1	0.90	0.37	65,65,65,65	0
56	MG	2A	3076	1/1	0.90	0.22	47,47,47,47	0
56	MG	1A	3796	1/1	0.90	0.18	73,73,73,73	0
56	MG	2A	3089	1/1	0.90	0.27	61,61,61,61	0
56	MG	2a	1713	1/1	0.90	0.14	72,72,72,72	0
56	MG	2A	3527	1/1	0.90	0.51	73,73,73,73	0
56	MG	2a	1716	1/1	0.90	0.11	85,85,85,85	0
56	MG	2a	1717	1/1	0.90	0.13	77,77,77,77	0
56	MG	2A	3528	1/1	0.90	0.12	64,64,64,64	0
56	MG	1A	3797	1/1	0.90	0.40	58,58,58,58	0
56	MG	1a	1921	1/1	0.90	0.08	68,68,68,68	0
56	MG	1a	1663	1/1	0.90	0.36	65,65,65,65	0
56	MG	1A	3451	1/1	0.90	0.14	42,42,42,42	0
56	MG	2A	3115	1/1	0.90	0.27	67,67,67,67	0
56	MG	1A	3513	1/1	0.90	0.16	32,32,32,32	0
56	MG	2A	3372	1/1	0.90	0.20	60,60,60,60	0
56	MG	2A	3124	1/1	0.90	0.31	45,45,45,45	0
56	MG	2A	3374	1/1	0.90	0.28	60,60,60,60	0
56	MG	1A	3801	1/1	0.90	0.13	63,63,63,63	0
56	MG	1A	3406	1/1	0.90	0.21	49,49,49,49	0
56	MG	1A	3707	1/1	0.90	0.11	50,50,50,50	0
56	MG	2a	1745	1/1	0.90	0.29	44,44,44,44	0
56	MG	1A	3408	1/1	0.90	0.12	74,74,74,74	0
56	MG	2A	3380	1/1	0.90	0.30	54,54,54,54	0
56	MG	2A	3551	1/1	0.90	0.15	59,59,59,59	0
56	MG	2A	3133	1/1	0.90	0.07	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3537	1/1	0.90	0.26	57,57,57,57	0
56	MG	2A	3388	1/1	0.90	0.12	53,53,53,53	0
56	MG	1a	1935	1/1	0.90	0.09	70,70,70,70	0
56	MG	2A	3394	1/1	0.90	0.26	59,59,59,59	0
56	MG	2A	3136	1/1	0.90	0.35	55,55,55,55	0
56	MG	1A	3251	1/1	0.90	0.28	49,49,49,49	0
56	MG	1a	1684	1/1	0.90	0.13	81,81,81,81	0
56	MG	1a	1807	1/1	0.90	0.13	76,76,76,76	0
56	MG	2A	3149	1/1	0.90	0.41	75,75,75,75	0
56	MG	1A	3635	1/1	0.90	0.25	69,69,69,69	0
56	MG	2A	3151	1/1	0.90	0.22	65,65,65,65	0
56	MG	1A	3101	1/1	0.90	0.78	45,45,45,45	0
56	MG	2A	3416	1/1	0.90	0.15	57,57,57,57	0
56	MG	1A	3904	1/1	0.90	0.31	41,41,41,41	0
56	MG	1A	3007	1/1	0.90	0.19	60,60,60,60	0
56	MG	1A	3906	1/1	0.90	0.83	53,53,53,53	0
56	MG	2A	3161	1/1	0.90	0.44	61,61,61,61	0
56	MG	2E	301	1/1	0.90	0.13	51,51,51,51	0
56	MG	1A	3204	1/1	0.90	0.17	61,61,61,61	0
56	MG	1A	3640	1/1	0.90	0.13	68,68,68,68	0
56	MG	1A	3466	1/1	0.90	0.11	45,45,45,45	0
56	MG	2A	3168	1/1	0.90	0.12	71,71,71,71	0
56	MG	1a	1840	1/1	0.90	0.09	70,70,70,70	0
56	MG	13	103	1/1	0.90	0.20	53,53,53,53	0
56	MG	1A	3386	1/1	0.90	0.22	54,54,54,54	0
56	MG	2T	201	1/1	0.90	0.14	55,55,55,55	0
56	MG	1A	3563	1/1	0.90	0.20	39,39,39,39	0
56	MG	2A	3191	1/1	0.90	0.13	50,50,50,50	0
56	MG	2a	1809	1/1	0.90	0.11	74,74,74,74	0
56	MG	1A	3255	1/1	0.90	0.57	44,44,44,44	0
56	MG	2a	1812	1/1	0.90	0.09	96,96,96,96	0
56	MG	2A	3194	1/1	0.90	0.36	47,47,47,47	0
56	MG	1A	3322	1/1	0.90	0.24	58,58,58,58	0
56	MG	1A	3073	1/1	0.90	0.11	46,46,46,46	0
56	MG	1o	103	1/1	0.90	0.09	75,75,75,75	0
56	MG	1A	3183	1/1	0.90	0.19	75,75,75,75	0
56	MG	2a	1607	1/1	0.90	0.08	83,83,83,83	0
56	MG	1A	3923	1/1	0.90	0.41	44,44,44,44	0
56	MG	1a	1729	1/1	0.90	0.19	53,53,53,53	0
56	MG	1A	3846	1/1	0.90	0.09	42,42,42,42	0
56	MG	1w	101	1/1	0.90	0.48	72,72,72,72	0
56	MG	1A	3162	1/1	0.90	0.45	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	1616	1/1	0.90	0.13	81,81,81,81	0
56	MG	2g	201	1/1	0.90	0.46	88,88,88,88	0
56	MG	1A	3293	1/1	0.90	0.27	38,38,38,38	0
56	MG	1A	3591	1/1	0.90	0.23	53,53,53,53	0
56	MG	1a	1739	1/1	0.90	0.08	75,75,75,75	0
56	MG	2A	3467	1/1	0.90	0.18	60,60,60,60	0
56	MG	1A	3341	1/1	0.90	0.26	46,46,46,46	0
56	MG	1A	3490	1/1	0.90	0.14	56,56,56,56	0
56	MG	2A	3270	1/1	0.90	0.26	64,64,64,64	0
57	KAN	2A	3569	33/33	0.90	0.16	56,65,71,73	0
56	MG	2A	3285	1/1	0.90	0.71	39,39,39,39	0
56	MG	1a	1622	1/1	0.91	0.41	56,56,56,56	0
56	MG	2a	1668	1/1	0.91	0.43	69,69,69,69	0
56	MG	1A	3026	1/1	0.91	0.13	32,32,32,32	0
56	MG	1A	3316	1/1	0.91	0.33	51,51,51,51	0
56	MG	1A	3844	1/1	0.91	0.56	79,79,79,79	0
56	MG	1A	3430	1/1	0.91	0.09	51,51,51,51	0
56	MG	2a	1674	1/1	0.91	0.12	90,90,90,90	0
56	MG	1A	3363	1/1	0.91	0.23	34,34,34,34	0
56	MG	1A	3777	1/1	0.91	0.17	63,63,63,63	0
56	MG	1a	1860	1/1	0.91	0.15	73,73,73,73	0
56	MG	1m	201	1/1	0.91	0.07	48,48,48,48	0
56	MG	1A	3780	1/1	0.91	0.20	70,70,70,70	0
56	MG	1A	3529	1/1	0.91	0.35	33,33,33,33	0
56	MG	1a	1864	1/1	0.91	0.15	55,55,55,55	0
56	MG	1a	1641	1/1	0.91	0.12	67,67,67,67	0
56	MG	2A	3383	1/1	0.91	0.20	43,43,43,43	0
56	MG	2A	3531	1/1	0.91	0.31	57,57,57,57	0
56	MG	1A	3643	1/1	0.91	0.19	54,54,54,54	0
56	MG	1Q	202	1/1	0.91	0.35	62,62,62,62	0
56	MG	1a	1652	1/1	0.91	0.23	57,57,57,57	0
56	MG	1A	3479	1/1	0.91	0.25	38,38,38,38	0
56	MG	1a	1874	1/1	0.91	0.10	71,71,71,71	0
56	MG	1A	3391	1/1	0.91	0.16	62,62,62,62	0
56	MG	2A	3544	1/1	0.91	0.13	69,69,69,69	0
56	MG	1a	1877	1/1	0.91	0.12	70,70,70,70	0
56	MG	2A	3398	1/1	0.91	0.37	76,76,76,76	0
56	MG	1U	201	1/1	0.91	0.73	41,41,41,41	0
56	MG	2A	3170	1/1	0.91	0.27	40,40,40,40	0
56	MG	2a	1711	1/1	0.91	0.07	81,81,81,81	0
56	MG	2A	3403	1/1	0.91	0.23	61,61,61,61	0
56	MG	1A	3366	1/1	0.91	0.33	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3410	1/1	0.91	0.39	50,50,50,50	0
56	MG	1A	3008	1/1	0.91	0.23	61,61,61,61	0
56	MG	2A	3553	1/1	0.91	0.33	67,67,67,67	0
56	MG	2A	3412	1/1	0.91	0.29	54,54,54,54	0
56	MG	2a	1720	1/1	0.91	0.24	60,60,60,60	0
56	MG	2A	3182	1/1	0.91	0.46	39,39,39,39	0
56	MG	1A	3924	1/1	0.91	0.38	52,52,52,52	0
56	MG	1A	3722	1/1	0.91	0.13	54,54,54,54	0
56	MG	1A	3074	1/1	0.91	0.16	50,50,50,50	0
56	MG	1A	3242	1/1	0.91	0.14	62,62,62,62	0
56	MG	2a	1727	1/1	0.91	0.36	97,97,97,97	0
56	MG	2a	1728	1/1	0.91	0.28	60,60,60,60	0
56	MG	2A	3419	1/1	0.91	0.24	62,62,62,62	0
56	MG	1x	116	1/1	0.91	0.12	78,78,78,78	0
56	MG	1A	3415	1/1	0.91	0.69	48,48,48,48	0
56	MG	2A	3567	1/1	0.91	0.20	67,67,67,67	0
56	MG	1a	1776	1/1	0.91	0.43	72,72,72,72	0
56	MG	1A	3740	1/1	0.91	0.10	52,52,52,52	0
56	MG	1a	1681	1/1	0.91	0.26	64,64,64,64	0
56	MG	2a	1742	1/1	0.91	0.29	51,51,51,51	0
56	MG	1A	3256	1/1	0.91	0.25	43,43,43,43	0
56	MG	2B	207	1/1	0.91	0.18	65,65,65,65	0
56	MG	2A	3003	1/1	0.91	0.19	60,60,60,60	0
56	MG	1A	3743	1/1	0.91	0.14	47,47,47,47	0
56	MG	1A	3260	1/1	0.91	0.34	25,25,25,25	0
56	MG	1A	3799	1/1	0.91	0.08	67,67,67,67	0
56	MG	2A	3253	1/1	0.91	0.35	50,50,50,50	0
56	MG	1a	1687	1/1	0.91	0.29	69,69,69,69	0
56	MG	2a	1766	1/1	0.91	0.08	73,73,73,73	0
56	MG	1A	3745	1/1	0.91	0.13	61,61,61,61	0
56	MG	1a	1689	1/1	0.91	0.22	48,48,48,48	0
56	MG	2A	3019	1/1	0.91	0.15	58,58,58,58	0
56	MG	2A	3453	1/1	0.91	0.15	74,74,74,74	0
56	MG	1A	3746	1/1	0.91	0.24	54,54,54,54	0
56	MG	2A	3280	1/1	0.91	0.26	36,36,36,36	0
56	MG	1A	3454	1/1	0.91	0.29	59,59,59,59	0
56	MG	2A	3286	1/1	0.91	0.35	50,50,50,50	0
56	MG	20	101	1/1	0.91	0.12	52,52,52,52	0
56	MG	1A	3133	1/1	0.91	0.83	54,54,54,54	0
56	MG	1a	1697	1/1	0.91	0.14	67,67,67,67	0
56	MG	2A	3030	1/1	0.91	0.11	56,56,56,56	0
56	MG	2a	1787	1/1	0.91	0.26	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	1789	1/1	0.91	0.14	66,66,66,66	0
56	MG	2A	3462	1/1	0.91	0.28	48,48,48,48	0
56	MG	1a	1916	1/1	0.91	0.34	70,70,70,70	0
56	MG	2A	3033	1/1	0.91	0.23	68,68,68,68	0
56	MG	2A	3034	1/1	0.91	0.32	55,55,55,55	0
56	MG	2A	3296	1/1	0.91	0.57	52,52,52,52	0
56	MG	1A	3625	1/1	0.91	0.28	57,57,57,57	0
56	MG	1A	3401	1/1	0.91	0.14	61,61,61,61	0
56	MG	2A	3039	1/1	0.91	0.30	41,41,41,41	0
56	MG	2A	3042	1/1	0.91	0.16	51,51,51,51	0
56	MG	1B	214	1/1	0.91	0.21	49,49,49,49	0
56	MG	2A	3044	1/1	0.91	0.49	49,49,49,49	0
56	MG	2A	3053	1/1	0.91	0.13	37,37,37,37	0
56	MG	2A	3324	1/1	0.91	0.17	68,68,68,68	0
56	MG	1A	3572	1/1	0.91	0.15	40,40,40,40	0
56	MG	2A	3055	1/1	0.91	0.32	69,69,69,69	0
56	MG	1A	3057	1/1	0.91	0.34	91,91,91,91	0
56	MG	1A	3577	1/1	0.91	0.39	51,51,51,51	0
56	MG	2a	1814	1/1	0.91	0.20	73,73,73,73	0
56	MG	2A	3330	1/1	0.91	0.13	62,62,62,62	0
56	MG	1A	3578	1/1	0.91	0.48	38,38,38,38	0
56	MG	1a	1927	1/1	0.91	0.09	70,70,70,70	0
56	MG	1A	3426	1/1	0.91	0.13	57,57,57,57	0
56	MG	1a	1718	1/1	0.91	0.20	73,73,73,73	0
56	MG	1a	1830	1/1	0.91	0.22	70,70,70,70	0
56	MG	1a	1933	1/1	0.91	0.09	74,74,74,74	0
56	MG	1a	1613	1/1	0.91	0.21	74,74,74,74	0
56	MG	2A	3094	1/1	0.91	0.16	61,61,61,61	0
56	MG	1A	3763	1/1	0.91	0.34	53,53,53,53	0
56	MG	1a	1834	1/1	0.91	0.19	64,64,64,64	0
56	MG	2A	3502	1/1	0.91	1.03	70,70,70,70	0
56	MG	2A	3109	1/1	0.91	0.38	57,57,57,57	0
56	MG	1A	3679	1/1	0.91	0.19	40,40,40,40	0
56	MG	1A	3688	1/1	0.91	0.11	37,37,37,37	0
56	MG	1A	3005	1/1	0.91	0.28	58,58,58,58	0
56	MG	2A	3507	1/1	0.91	0.47	57,57,57,57	0
56	MG	1a	1731	1/1	0.91	0.12	72,72,72,72	0
56	MG	1a	1843	1/1	0.91	0.23	63,63,63,63	0
56	MG	1a	1733	1/1	0.91	0.04	88,88,88,88	0
56	MG	1A	3691	1/1	0.91	0.23	37,37,37,37	0
56	MG	1A	3278	1/1	0.92	0.11	39,39,39,39	0
56	MG	1A	3423	1/1	0.92	0.10	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3463	1/1	0.92	0.16	66,66,66,66	0
56	MG	1x	106	1/1	0.92	0.18	64,64,64,64	0
56	MG	2A	3239	1/1	0.92	0.25	40,40,40,40	0
56	MG	2A	3240	1/1	0.92	0.24	50,50,50,50	0
56	MG	1a	1714	1/1	0.92	0.26	80,80,80,80	0
56	MG	1A	3909	1/1	0.92	0.23	75,75,75,75	0
56	MG	1A	3160	1/1	0.92	0.08	76,76,76,76	0
56	MG	1x	112	1/1	0.92	0.20	72,72,72,72	0
56	MG	1A	3912	1/1	0.92	0.12	61,61,61,61	0
56	MG	1a	1719	1/1	0.92	0.11	95,95,95,95	0
56	MG	1a	1720	1/1	0.92	0.14	80,80,80,80	0
56	MG	15	102	1/1	0.92	0.51	39,39,39,39	0
56	MG	2A	3477	1/1	0.92	0.25	58,58,58,58	0
56	MG	1A	3913	1/1	0.92	0.19	65,65,65,65	0
56	MG	1A	3395	1/1	0.92	0.15	70,70,70,70	0
56	MG	1A	3198	1/1	0.92	0.58	52,52,52,52	0
56	MG	1A	3290	1/1	0.92	0.42	40,40,40,40	0
56	MG	1A	3824	1/1	0.92	0.15	62,62,62,62	0
56	MG	1a	1875	1/1	0.92	0.20	60,60,60,60	0
56	MG	1A	3127	1/1	0.92	0.21	57,57,57,57	0
56	MG	2A	3014	1/1	0.92	0.23	51,51,51,51	0
56	MG	1A	3486	1/1	0.92	0.10	50,50,50,50	0
56	MG	1A	3834	1/1	0.92	0.09	68,68,68,68	0
56	MG	2a	1673	1/1	0.92	0.08	88,88,88,88	0
56	MG	1A	3748	1/1	0.92	0.21	47,47,47,47	0
56	MG	1A	3033	1/1	0.92	0.14	68,68,68,68	0
56	MG	1A	3583	1/1	0.92	0.37	39,39,39,39	0
56	MG	2A	3022	1/1	0.92	0.10	36,36,36,36	0
56	MG	1A	3585	1/1	0.92	0.37	28,28,28,28	0
56	MG	1A	3035	1/1	0.92	0.26	39,39,39,39	0
56	MG	1a	1743	1/1	0.92	0.34	66,66,66,66	0
56	MG	2A	3312	1/1	0.92	0.26	75,75,75,75	0
56	MG	1a	1886	1/1	0.92	0.10	81,81,81,81	0
56	MG	1A	3491	1/1	0.92	0.26	56,56,56,56	0
56	MG	2a	1690	1/1	0.92	0.27	90,90,90,90	0
56	MG	1A	3649	1/1	0.92	0.11	65,65,65,65	0
56	MG	1A	3130	1/1	0.92	0.39	54,54,54,54	0
56	MG	1A	3434	1/1	0.92	0.34	78,78,78,78	0
56	MG	1A	3592	1/1	0.92	0.21	48,48,48,48	0
56	MG	1a	1895	1/1	0.92	0.45	51,51,51,51	0
56	MG	1a	1617	1/1	0.92	0.03	84,84,84,84	0
56	MG	1A	3435	1/1	0.92	0.32	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3597	1/1	0.92	0.35	45,45,45,45	0
56	MG	2A	3047	1/1	0.92	0.27	46,46,46,46	0
56	MG	2A	3338	1/1	0.92	0.36	53,53,53,53	0
56	MG	1A	3370	1/1	0.92	0.20	33,33,33,33	0
56	MG	2A	3521	1/1	0.92	0.32	45,45,45,45	0
56	MG	2a	1709	1/1	0.92	0.25	70,70,70,70	0
56	MG	1A	3661	1/1	0.92	0.06	70,70,70,70	0
56	MG	1A	3301	1/1	0.92	0.20	42,42,42,42	0
56	MG	2A	3056	1/1	0.92	0.15	58,58,58,58	0
56	MG	1A	3244	1/1	0.92	0.20	53,53,53,53	0
56	MG	1A	3502	1/1	0.92	0.14	52,52,52,52	0
56	MG	1a	1765	1/1	0.92	0.10	88,88,88,88	0
56	MG	2A	3065	1/1	0.92	0.09	79,79,79,79	0
56	MG	1A	3147	1/1	0.92	0.19	59,59,59,59	0
56	MG	1B	215	1/1	0.92	0.16	53,53,53,53	0
56	MG	1a	1772	1/1	0.92	0.08	58,58,58,58	0
56	MG	2A	3357	1/1	0.92	0.19	51,51,51,51	0
56	MG	2A	3533	1/1	0.92	0.08	64,64,64,64	0
56	MG	2A	3535	1/1	0.92	0.19	65,65,65,65	0
56	MG	2A	3082	1/1	0.92	0.19	63,63,63,63	0
56	MG	1a	1630	1/1	0.92	0.10	49,49,49,49	0
56	MG	2A	3362	1/1	0.92	0.29	58,58,58,58	0
56	MG	2A	3540	1/1	0.92	0.08	84,84,84,84	0
56	MG	1A	3608	1/1	0.92	0.35	57,57,57,57	0
56	MG	2A	3090	1/1	0.92	0.08	54,54,54,54	0
56	MG	2A	3367	1/1	0.92	0.37	69,69,69,69	0
56	MG	1A	3609	1/1	0.92	0.22	57,57,57,57	0
56	MG	1a	1634	1/1	0.92	0.15	61,61,61,61	0
56	MG	2A	3096	1/1	0.92	0.19	44,44,44,44	0
56	MG	2A	3098	1/1	0.92	0.26	74,74,74,74	0
56	MG	1A	3778	1/1	0.92	0.49	64,64,64,64	0
56	MG	1A	3446	1/1	0.92	0.24	47,47,47,47	0
56	MG	1A	3674	1/1	0.92	0.19	37,37,37,37	0
56	MG	1A	3096	1/1	0.92	0.36	59,59,59,59	0
56	MG	2A	3113	1/1	0.92	0.18	72,72,72,72	0
56	MG	1A	3683	1/1	0.92	0.28	54,54,54,54	0
56	MG	2a	1762	1/1	0.92	0.29	62,62,62,62	0
56	MG	2a	1763	1/1	0.92	0.17	55,55,55,55	0
56	MG	2A	3118	1/1	0.92	0.42	42,42,42,42	0
56	MG	1A	3612	1/1	0.92	0.13	53,53,53,53	0
56	MG	2A	3381	1/1	0.92	0.07	59,59,59,59	0
56	MG	1a	1784	1/1	0.92	0.07	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	1769	1/1	0.92	0.23	70,70,70,70	0
56	MG	2A	3125	1/1	0.92	0.24	69,69,69,69	0
56	MG	2A	3127	1/1	0.92	0.26	76,76,76,76	0
56	MG	1B	226	1/1	0.92	0.13	53,53,53,53	0
56	MG	1B	227	1/1	0.92	0.10	58,58,58,58	0
56	MG	1A	3080	1/1	0.92	0.21	57,57,57,57	0
56	MG	2a	1779	1/1	0.92	0.08	81,81,81,81	0
56	MG	1A	3102	1/1	0.92	0.37	30,30,30,30	0
56	MG	1a	1939	1/1	0.92	0.29	68,68,68,68	0
56	MG	2A	3397	1/1	0.92	0.09	74,74,74,74	0
56	MG	1a	1940	1/1	0.92	0.21	47,47,47,47	0
56	MG	1D	301	1/1	0.92	0.36	28,28,28,28	0
56	MG	1a	1670	1/1	0.92	0.41	62,62,62,62	0
56	MG	2A	3137	1/1	0.92	0.25	57,57,57,57	0
56	MG	1A	3013	1/1	0.92	0.23	46,46,46,46	0
56	MG	2B	213	1/1	0.92	0.18	78,78,78,78	0
56	MG	2A	3409	1/1	0.92	0.19	68,68,68,68	0
56	MG	2D	303	1/1	0.92	0.18	67,67,67,67	0
56	MG	2a	1796	1/1	0.92	0.12	68,68,68,68	0
56	MG	2A	3142	1/1	0.92	0.13	73,73,73,73	0
56	MG	1a	1946	1/1	0.92	0.11	69,69,69,69	0
56	MG	1A	3698	1/1	0.92	0.13	21,21,21,21	0
56	MG	1A	3879	1/1	0.92	0.14	68,68,68,68	0
56	MG	1A	3518	1/1	0.92	0.22	45,45,45,45	0
56	MG	1A	3105	1/1	0.92	0.44	41,41,41,41	0
56	MG	1a	1954	1/1	0.92	0.14	70,70,70,70	0
56	MG	1A	3623	1/1	0.92	0.24	49,49,49,49	0
56	MG	1a	1809	1/1	0.92	0.11	63,63,63,63	0
56	MG	2a	1808	1/1	0.92	0.14	77,77,77,77	0
56	MG	1A	3068	1/1	0.92	0.21	62,62,62,62	0
56	MG	1A	3458	1/1	0.92	1.22	54,54,54,54	0
56	MG	1N	202	1/1	0.92	0.39	71,71,71,71	0
56	MG	1l	201	1/1	0.92	0.12	58,58,58,58	0
56	MG	1A	3414	1/1	0.92	0.34	54,54,54,54	0
56	MG	2a	1601	1/1	0.92	0.26	76,76,76,76	0
56	MG	1O	3102	1/1	0.92	0.16	60,60,60,60	0
56	MG	2A	3437	1/1	0.92	0.26	58,58,58,58	0
56	MG	1P	201	1/1	0.92	0.32	49,49,49,49	0
56	MG	1A	3223	1/1	0.92	0.60	30,30,30,30	0
56	MG	1A	3051	1/1	0.92	0.14	27,27,27,27	0
56	MG	2A	3172	1/1	0.92	0.39	48,48,48,48	0
56	MG	1A	3004	1/1	0.92	0.11	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3178	1/1	0.92	0.49	35,35,35,35	0
56	MG	1A	3802	1/1	0.92	0.10	65,65,65,65	0
56	MG	1A	3721	1/1	0.92	0.22	33,33,33,33	0
56	MG	2A	3450	1/1	0.92	0.20	66,66,66,66	0
56	MG	1a	1842	1/1	0.92	0.23	55,55,55,55	0
56	MG	1V	201	1/1	0.92	0.26	43,43,43,43	0
56	MG	1a	1699	1/1	0.92	0.30	64,64,64,64	0
56	MG	1A	3903	1/1	0.92	0.29	39,39,39,39	0
56	MG	2A	3203	1/1	0.92	0.21	48,48,48,48	0
56	MG	1a	1707	1/1	0.92	0.48	41,41,41,41	0
56	MG	2x	104	1/1	0.92	0.18	68,68,68,68	0
56	MG	1A	3392	1/1	0.92	0.39	49,49,49,49	0
56	MG	2a	1630	1/1	0.92	0.20	57,57,57,57	0
58	ZN	14	501	1/1	0.92	0.05	99,99,99,99	0
56	MG	1A	3634	1/1	0.92	0.09	64,64,64,64	0
56	MG	1A	3907	1/1	0.93	0.06	45,45,45,45	0
56	MG	1A	3600	1/1	0.93	0.32	52,52,52,52	0
56	MG	2A	3468	1/1	0.93	0.39	73,73,73,73	0
56	MG	2A	3277	1/1	0.93	0.08	58,58,58,58	0
56	MG	1A	3795	1/1	0.93	0.31	69,69,69,69	0
56	MG	1A	3031	1/1	0.93	0.12	36,36,36,36	0
56	MG	1A	3911	1/1	0.93	0.11	49,49,49,49	0
56	MG	2A	3025	1/1	0.93	0.39	54,54,54,54	0
56	MG	2a	1651	1/1	0.93	0.27	46,46,46,46	0
56	MG	2A	3288	1/1	0.93	0.30	74,74,74,74	0
56	MG	2A	3026	1/1	0.93	0.22	39,39,39,39	0
56	MG	1a	1601	1/1	0.93	0.26	59,59,59,59	0
56	MG	2a	1659	1/1	0.93	0.10	69,69,69,69	0
56	MG	2A	3479	1/1	0.93	0.29	46,46,46,46	0
56	MG	1A	3389	1/1	0.93	0.21	65,65,65,65	0
56	MG	1A	3497	1/1	0.93	0.14	59,59,59,59	0
56	MG	2A	3483	1/1	0.93	0.32	75,75,75,75	0
56	MG	1A	3692	1/1	0.93	0.18	29,29,29,29	0
56	MG	2A	3488	1/1	0.93	0.30	61,61,61,61	0
56	MG	1A	3025	1/1	0.93	0.17	41,41,41,41	0
56	MG	1A	3078	1/1	0.93	0.20	14,14,14,14	0
56	MG	1A	3257	1/1	0.93	0.20	57,57,57,57	0
56	MG	2A	3037	1/1	0.93	0.13	59,59,59,59	0
56	MG	1A	3324	1/1	0.93	0.26	49,49,49,49	0
56	MG	1a	1893	1/1	0.93	0.32	79,79,79,79	0
56	MG	1A	3804	1/1	0.93	0.17	77,77,77,77	0
56	MG	2a	1676	1/1	0.93	0.14	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3306	1/1	0.93	0.20	74,74,74,74	0
56	MG	2A	3307	1/1	0.93	0.16	75,75,75,75	0
56	MG	1A	3326	1/1	0.93	0.27	42,42,42,42	0
56	MG	1A	3176	1/1	0.93	0.41	77,77,77,77	0
56	MG	2A	3322	1/1	0.93	0.63	54,54,54,54	0
56	MG	1a	1614	1/1	0.93	0.12	47,47,47,47	0
56	MG	1A	3132	1/1	0.93	0.31	33,33,33,33	0
56	MG	1a	1904	1/1	0.93	0.47	70,70,70,70	0
56	MG	1A	3265	1/1	0.93	0.29	41,41,41,41	0
56	MG	1A	3272	1/1	0.93	0.22	27,27,27,27	0
56	MG	1A	3443	1/1	0.93	0.32	35,35,35,35	0
56	MG	2A	3331	1/1	0.93	0.32	56,56,56,56	0
56	MG	1A	3713	1/1	0.93	0.12	61,61,61,61	0
56	MG	1A	3930	1/1	0.93	0.15	49,49,49,49	0
56	MG	2A	3064	1/1	0.93	0.29	59,59,59,59	0
56	MG	1A	3818	1/1	0.93	0.32	52,52,52,52	0
56	MG	1A	3821	1/1	0.93	0.32	30,30,30,30	0
56	MG	1A	3015	1/1	0.93	0.11	53,53,53,53	0
56	MG	1A	3717	1/1	0.93	0.15	62,62,62,62	0
56	MG	1A	3521	1/1	0.93	0.38	31,31,31,31	0
56	MG	1A	3525	1/1	0.93	0.38	34,34,34,34	0
56	MG	1a	1775	1/1	0.93	0.18	62,62,62,62	0
56	MG	1A	3626	1/1	0.93	0.63	47,47,47,47	0
56	MG	1a	1631	1/1	0.93	0.10	64,64,64,64	0
56	MG	2A	3092	1/1	0.93	0.27	55,55,55,55	0
56	MG	2A	3352	1/1	0.93	0.06	70,70,70,70	0
56	MG	2a	1714	1/1	0.93	0.36	58,58,58,58	0
56	MG	1A	3181	1/1	0.93	0.13	60,60,60,60	0
56	MG	1a	1928	1/1	0.93	0.30	70,70,70,70	0
56	MG	1A	3344	1/1	0.93	0.41	36,36,36,36	0
56	MG	2A	3099	1/1	0.93	0.19	46,46,46,46	0
56	MG	2A	3359	1/1	0.93	0.09	54,54,54,54	0
56	MG	2A	3101	1/1	0.93	0.20	41,41,41,41	0
56	MG	1a	1930	1/1	0.93	0.12	72,72,72,72	0
56	MG	2A	3107	1/1	0.93	0.14	60,60,60,60	0
56	MG	1A	3739	1/1	0.93	0.19	48,48,48,48	0
56	MG	1B	211	1/1	0.93	0.46	42,42,42,42	0
56	MG	1A	3347	1/1	0.93	0.30	31,31,31,31	0
56	MG	1A	3535	1/1	0.93	0.50	44,44,44,44	0
56	MG	1A	3631	1/1	0.93	0.15	77,77,77,77	0
56	MG	2A	3117	1/1	0.93	0.35	32,32,32,32	0
56	MG	1A	3348	1/1	0.93	0.34	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3107	1/1	0.93	0.44	30,30,30,30	0
56	MG	2a	1733	1/1	0.93	0.47	74,74,74,74	0
56	MG	1A	3539	1/1	0.93	0.25	33,33,33,33	0
56	MG	1a	1788	1/1	0.93	0.08	71,71,71,71	0
56	MG	2A	3126	1/1	0.93	0.22	53,53,53,53	0
56	MG	1a	1660	1/1	0.93	0.28	47,47,47,47	0
56	MG	1a	1790	1/1	0.93	0.11	69,69,69,69	0
56	MG	1a	1791	1/1	0.93	0.27	69,69,69,69	0
56	MG	1A	3456	1/1	0.93	0.23	44,44,44,44	0
56	MG	2A	3131	1/1	0.93	0.25	58,58,58,58	0
56	MG	1A	3550	1/1	0.93	0.44	29,29,29,29	0
56	MG	2A	3385	1/1	0.93	0.20	51,51,51,51	0
56	MG	1A	3233	1/1	0.93	0.13	48,48,48,48	0
56	MG	1A	3639	1/1	0.93	0.12	29,29,29,29	0
56	MG	1a	1668	1/1	0.93	0.36	62,62,62,62	0
56	MG	1A	3361	1/1	0.93	0.45	30,30,30,30	0
56	MG	1A	3857	1/1	0.93	0.16	59,59,59,59	0
56	MG	2A	3562	1/1	0.93	0.16	73,73,73,73	0
56	MG	1A	3753	1/1	0.93	0.22	57,57,57,57	0
56	MG	1A	3459	1/1	0.93	0.32	57,57,57,57	0
56	MG	1a	1811	1/1	0.93	0.49	63,63,63,63	0
56	MG	1A	3135	1/1	0.93	0.47	48,48,48,48	0
56	MG	2B	201	1/1	0.93	0.08	75,75,75,75	0
56	MG	1A	3756	1/1	0.93	0.12	67,67,67,67	0
56	MG	1a	1816	1/1	0.93	0.16	81,81,81,81	0
56	MG	1A	3561	1/1	0.93	0.49	28,28,28,28	0
56	MG	2A	3405	1/1	0.93	0.37	58,58,58,58	0
56	MG	2A	3407	1/1	0.93	0.18	59,59,59,59	0
56	MG	1a	1824	1/1	0.93	0.12	80,80,80,80	0
56	MG	1A	3364	1/1	0.93	0.36	49,49,49,49	0
56	MG	1A	3759	1/1	0.93	0.14	73,73,73,73	0
56	MG	1A	3760	1/1	0.93	0.44	52,52,52,52	0
56	MG	1q	201	1/1	0.93	0.22	66,66,66,66	0
56	MG	1A	3237	1/1	0.93	0.13	56,56,56,56	0
56	MG	1A	3565	1/1	0.93	0.39	60,60,60,60	0
56	MG	1a	1836	1/1	0.93	0.22	72,72,72,72	0
56	MG	1A	3205	1/1	0.93	0.76	65,65,65,65	0
56	MG	1A	3470	1/1	0.93	0.64	43,43,43,43	0
56	MG	1A	3768	1/1	0.93	0.10	71,71,71,71	0
56	MG	2A	3421	1/1	0.93	0.32	59,59,59,59	0
56	MG	1A	3150	1/1	0.93	0.33	75,75,75,75	0
56	MG	1A	3475	1/1	0.93	0.19	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3110	1/1	0.93	0.22	68,68,68,68	0
56	MG	2A	3429	1/1	0.93	0.20	74,74,74,74	0
56	MG	2W	201	1/1	0.93	0.44	76,76,76,76	0
56	MG	1P	202	1/1	0.93	0.33	69,69,69,69	0
56	MG	2A	3179	1/1	0.93	0.27	51,51,51,51	0
56	MG	2A	3435	1/1	0.93	0.21	74,74,74,74	0
56	MG	1A	3579	1/1	0.93	0.34	41,41,41,41	0
56	MG	26	101	1/1	0.93	0.11	61,61,61,61	0
56	MG	1a	1701	1/1	0.93	0.36	47,47,47,47	0
56	MG	1A	3582	1/1	0.93	0.36	49,49,49,49	0
56	MG	1A	3209	1/1	0.93	0.75	44,44,44,44	0
56	MG	1A	3417	1/1	0.93	0.32	51,51,51,51	0
56	MG	1A	3069	1/1	0.93	0.21	62,62,62,62	0
56	MG	1A	3663	1/1	0.93	0.37	54,54,54,54	0
56	MG	1A	3664	1/1	0.93	0.17	59,59,59,59	0
56	MG	1x	118	1/1	0.93	0.16	71,71,71,71	0
56	MG	1A	3304	1/1	0.93	0.29	46,46,46,46	0
56	MG	2a	1612	1/1	0.93	0.16	68,68,68,68	0
56	MG	2A	3227	1/1	0.93	0.38	37,37,37,37	0
56	MG	2a	1614	1/1	0.93	0.14	84,84,84,84	0
56	MG	1A	3588	1/1	0.93	0.53	46,46,46,46	0
56	MG	2A	3452	1/1	0.93	0.24	59,59,59,59	0
56	MG	1X	101	1/1	0.93	0.19	56,56,56,56	0
56	MG	1A	3382	1/1	0.93	0.39	56,56,56,56	0
56	MG	1A	3383	1/1	0.93	0.21	59,59,59,59	0
56	MG	1A	3092	1/1	0.93	0.47	54,54,54,54	0
56	MG	1a	1722	1/1	0.93	0.18	85,85,85,85	0
56	MG	1A	3001	1/1	0.93	0.33	39,39,39,39	0
56	MG	1A	3425	1/1	0.93	0.35	46,46,46,46	0
56	MG	2A	3013	1/1	0.93	0.09	60,60,60,60	0
56	MG	1A	3310	1/1	0.93	0.19	53,53,53,53	0
57	KAN	1A	3933	33/33	0.93	0.18	34,44,58,64	0
57	KAN	2A	3568	33/33	0.93	0.17	51,58,63,65	0
56	MG	15	103	1/1	0.93	0.44	77,77,77,77	0
57	KAN	2a	1828	33/33	0.93	0.17	47,61,67,70	0
56	MG	1A	3098	1/1	0.93	0.09	48,48,48,48	0
58	ZN	2Y	501	1/1	0.93	0.12	98,98,98,98	0
56	MG	2A	3264	1/1	0.93	0.35	37,37,37,37	0
56	MG	2A	3423	1/1	0.94	0.10	88,88,88,88	0
56	MG	1a	1695	1/1	0.94	0.45	48,48,48,48	0
56	MG	1A	3882	1/1	0.94	0.15	72,72,72,72	0
56	MG	1A	3473	1/1	0.94	0.09	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3541	1/1	0.94	0.39	43,43,43,43	0
56	MG	1A	3097	1/1	0.94	0.38	55,55,55,55	0
56	MG	1x	105	1/1	0.94	0.33	41,41,41,41	0
56	MG	1a	1702	1/1	0.94	0.36	58,58,58,58	0
56	MG	1A	3702	1/1	0.94	0.15	31,31,31,31	0
56	MG	2A	3183	1/1	0.94	0.29	61,61,61,61	0
56	MG	2A	3187	1/1	0.94	0.47	39,39,39,39	0
56	MG	1A	3545	1/1	0.94	0.27	31,31,31,31	0
56	MG	2a	1625	1/1	0.94	0.31	51,51,51,51	0
56	MG	2a	1629	1/1	0.94	0.08	55,55,55,55	0
56	MG	1x	110	1/1	0.94	0.20	68,68,68,68	0
56	MG	2A	3444	1/1	0.94	0.19	55,55,55,55	0
56	MG	1a	1848	1/1	0.94	0.29	56,56,56,56	0
56	MG	2a	1635	1/1	0.94	0.52	59,59,59,59	0
56	MG	1A	3890	1/1	0.94	0.08	69,69,69,69	0
56	MG	2A	3195	1/1	0.94	0.24	53,53,53,53	0
56	MG	1A	3548	1/1	0.94	0.29	54,54,54,54	0
56	MG	2A	3198	1/1	0.94	0.42	50,50,50,50	0
56	MG	1A	3027	1/1	0.94	0.12	28,28,28,28	0
56	MG	2A	3207	1/1	0.94	0.46	34,34,34,34	0
56	MG	2A	3210	1/1	0.94	0.37	44,44,44,44	0
56	MG	1A	3552	1/1	0.94	0.27	34,34,34,34	0
56	MG	1A	3894	1/1	0.94	0.14	53,53,53,53	0
56	MG	1a	1715	1/1	0.94	0.46	58,58,58,58	0
56	MG	2A	3223	1/1	0.94	0.29	38,38,38,38	0
56	MG	2a	1654	1/1	0.94	0.27	76,76,76,76	0
56	MG	1x	121	1/1	0.94	0.13	57,57,57,57	0
56	MG	11	101	1/1	0.94	0.42	69,69,69,69	0
56	MG	2a	1657	1/1	0.94	0.29	60,60,60,60	0
56	MG	1A	3895	1/1	0.94	0.12	57,57,57,57	0
56	MG	1A	3125	1/1	0.94	0.32	59,59,59,59	0
56	MG	2a	1660	1/1	0.94	0.10	57,57,57,57	0
56	MG	2A	3238	1/1	0.94	0.49	48,48,48,48	0
56	MG	1A	3901	1/1	0.94	0.16	53,53,53,53	0
56	MG	1A	3710	1/1	0.94	0.14	43,43,43,43	0
56	MG	1A	3356	1/1	0.94	0.43	26,26,26,26	0
56	MG	2a	1665	1/1	0.94	0.27	61,61,61,61	0
56	MG	2A	3010	1/1	0.94	0.34	49,49,49,49	0
56	MG	1A	3060	1/1	0.94	0.12	29,29,29,29	0
56	MG	2A	3251	1/1	0.94	0.49	48,48,48,48	0
56	MG	1A	3248	1/1	0.94	0.23	66,66,66,66	0
56	MG	2A	3254	1/1	0.94	0.35	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3213	1/1	0.94	0.28	57,57,57,57	0
56	MG	2A	3015	1/1	0.94	0.07	51,51,51,51	0
56	MG	1a	1727	1/1	0.94	0.14	65,65,65,65	0
56	MG	2A	3475	1/1	0.94	0.12	62,62,62,62	0
56	MG	1a	1873	1/1	0.94	0.13	62,62,62,62	0
56	MG	2A	3267	1/1	0.94	0.49	33,33,33,33	0
56	MG	2A	3478	1/1	0.94	0.19	64,64,64,64	0
56	MG	1A	3720	1/1	0.94	0.16	66,66,66,66	0
56	MG	1A	3562	1/1	0.94	0.51	28,28,28,28	0
56	MG	2a	1682	1/1	0.94	0.07	80,80,80,80	0
56	MG	2A	3276	1/1	0.94	0.32	37,37,37,37	0
56	MG	1A	3484	1/1	0.94	0.27	51,51,51,51	0
56	MG	1a	1732	1/1	0.94	0.16	53,53,53,53	0
56	MG	2A	3487	1/1	0.94	0.32	41,41,41,41	0
56	MG	1A	3723	1/1	0.94	0.13	66,66,66,66	0
56	MG	1a	1734	1/1	0.94	0.45	76,76,76,76	0
56	MG	1A	3807	1/1	0.94	0.11	51,51,51,51	0
56	MG	1a	1603	1/1	0.94	0.20	61,61,61,61	0
56	MG	1A	3725	1/1	0.94	0.16	27,27,27,27	0
56	MG	2A	3029	1/1	0.94	0.12	67,67,67,67	0
56	MG	1A	3173	1/1	0.94	0.07	70,70,70,70	0
56	MG	2A	3292	1/1	0.94	0.47	50,50,50,50	0
56	MG	1A	3216	1/1	0.94	0.70	49,49,49,49	0
56	MG	1A	3813	1/1	0.94	0.14	42,42,42,42	0
56	MG	1A	3487	1/1	0.94	0.34	52,52,52,52	0
56	MG	1A	3734	1/1	0.94	0.24	40,40,40,40	0
56	MG	1A	3568	1/1	0.94	0.37	42,42,42,42	0
56	MG	2a	1706	1/1	0.94	0.09	57,57,57,57	0
56	MG	1A	3064	1/1	0.94	0.15	36,36,36,36	0
56	MG	1A	3575	1/1	0.94	0.46	31,31,31,31	0
56	MG	2a	1710	1/1	0.94	0.08	85,85,85,85	0
56	MG	2A	3041	1/1	0.94	0.24	39,39,39,39	0
56	MG	1A	3439	1/1	0.94	0.07	44,44,44,44	0
56	MG	1A	3825	1/1	0.94	0.23	45,45,45,45	0
56	MG	1a	1750	1/1	0.94	0.28	70,70,70,70	0
56	MG	2A	3308	1/1	0.94	0.38	58,58,58,58	0
56	MG	1a	1751	1/1	0.94	0.10	62,62,62,62	0
56	MG	1a	1753	1/1	0.94	0.15	58,58,58,58	0
56	MG	2a	1718	1/1	0.94	0.09	68,68,68,68	0
56	MG	2A	3317	1/1	0.94	0.38	38,38,38,38	0
56	MG	2A	3511	1/1	0.94	0.51	87,87,87,87	0
56	MG	1a	1900	1/1	0.94	0.23	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3826	1/1	0.94	0.19	82,82,82,82	0
56	MG	1a	1902	1/1	0.94	0.37	85,85,85,85	0
56	MG	1A	3066	1/1	0.94	0.08	38,38,38,38	0
56	MG	2A	3516	1/1	0.94	0.09	78,78,78,78	0
56	MG	2A	3058	1/1	0.94	0.52	55,55,55,55	0
56	MG	2A	3519	1/1	0.94	0.39	56,56,56,56	0
56	MG	1a	1757	1/1	0.94	0.34	69,69,69,69	0
56	MG	1A	3089	1/1	0.94	0.11	32,32,32,32	0
56	MG	1A	3493	1/1	0.94	0.11	52,52,52,52	0
56	MG	1a	1909	1/1	0.94	0.27	62,62,62,62	0
56	MG	1A	3106	1/1	0.94	0.39	31,31,31,31	0
56	MG	2a	1736	1/1	0.94	0.07	64,64,64,64	0
56	MG	2A	3071	1/1	0.94	0.19	72,72,72,72	0
56	MG	2A	3074	1/1	0.94	0.24	51,51,51,51	0
56	MG	1A	3445	1/1	0.94	0.44	51,51,51,51	0
56	MG	2a	1741	1/1	0.94	0.51	50,50,50,50	0
56	MG	1A	3225	1/1	0.94	0.28	40,40,40,40	0
56	MG	2a	1743	1/1	0.94	0.51	39,39,39,39	0
56	MG	2A	3080	1/1	0.94	0.30	45,45,45,45	0
56	MG	2a	1746	1/1	0.94	0.18	77,77,77,77	0
56	MG	1A	3841	1/1	0.94	0.16	73,73,73,73	0
56	MG	2a	1748	1/1	0.94	0.24	69,69,69,69	0
56	MG	2A	3343	1/1	0.94	0.32	67,67,67,67	0
56	MG	2A	3083	1/1	0.94	0.17	69,69,69,69	0
56	MG	2A	3085	1/1	0.94	0.20	67,67,67,67	0
56	MG	2A	3534	1/1	0.94	0.17	57,57,57,57	0
56	MG	2a	1759	1/1	0.94	0.06	63,63,63,63	0
56	MG	1A	3651	1/1	0.94	0.20	58,58,58,58	0
56	MG	2a	1761	1/1	0.94	0.11	69,69,69,69	0
56	MG	2A	3087	1/1	0.94	0.18	76,76,76,76	0
56	MG	2A	3349	1/1	0.94	0.20	48,48,48,48	0
56	MG	2A	3088	1/1	0.94	0.24	49,49,49,49	0
56	MG	1A	3179	1/1	0.94	0.06	70,70,70,70	0
56	MG	2A	3541	1/1	0.94	0.10	85,85,85,85	0
56	MG	1A	3319	1/1	0.94	0.41	44,44,44,44	0
56	MG	1a	1770	1/1	0.94	0.08	60,60,60,60	0
56	MG	1A	3020	1/1	0.94	0.12	47,47,47,47	0
56	MG	1A	3109	1/1	0.94	0.28	47,47,47,47	0
56	MG	1A	3269	1/1	0.94	0.31	33,33,33,33	0
56	MG	1A	3659	1/1	0.94	0.16	65,65,65,65	0
56	MG	2a	1777	1/1	0.94	0.10	85,85,85,85	0
56	MG	1A	3416	1/1	0.94	0.11	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1B	213	1/1	0.94	0.20	40,40,40,40	0
56	MG	1A	3852	1/1	0.94	0.12	61,61,61,61	0
56	MG	2A	3364	1/1	0.94	0.47	62,62,62,62	0
56	MG	1a	1640	1/1	0.94	0.34	55,55,55,55	0
56	MG	2a	1784	1/1	0.94	0.20	66,66,66,66	0
56	MG	1A	3021	1/1	0.94	0.20	40,40,40,40	0
56	MG	1a	1644	1/1	0.94	0.22	63,63,63,63	0
56	MG	1a	1646	1/1	0.94	0.20	67,67,67,67	0
56	MG	1A	3509	1/1	0.94	0.21	52,52,52,52	0
56	MG	2a	1790	1/1	0.94	0.12	92,92,92,92	0
56	MG	2A	3114	1/1	0.94	0.39	60,60,60,60	0
56	MG	2A	3558	1/1	0.94	0.38	46,46,46,46	0
56	MG	1A	3328	1/1	0.94	0.25	46,46,46,46	0
56	MG	1A	3762	1/1	0.94	0.12	57,57,57,57	0
56	MG	1A	3511	1/1	0.94	0.11	49,49,49,49	0
56	MG	2A	3122	1/1	0.94	0.32	33,33,33,33	0
56	MG	1a	1654	1/1	0.94	0.32	41,41,41,41	0
56	MG	1A	3764	1/1	0.94	0.18	64,64,64,64	0
56	MG	1A	3666	1/1	0.94	0.21	80,80,80,80	0
56	MG	1a	1943	1/1	0.94	0.27	69,69,69,69	0
56	MG	1A	3861	1/1	0.94	0.09	81,81,81,81	0
56	MG	2A	3382	1/1	0.94	0.17	84,84,84,84	0
56	MG	2a	1804	1/1	0.94	0.15	78,78,78,78	0
56	MG	1A	3042	1/1	0.94	0.24	42,42,42,42	0
56	MG	1A	3232	1/1	0.94	0.28	58,58,58,58	0
56	MG	1A	3669	1/1	0.94	0.16	62,62,62,62	0
56	MG	1A	3337	1/1	0.94	0.25	42,42,42,42	0
56	MG	1a	1952	1/1	0.94	0.04	58,58,58,58	0
56	MG	2A	3390	1/1	0.94	0.30	72,72,72,72	0
56	MG	1a	1798	1/1	0.94	0.11	75,75,75,75	0
56	MG	2A	3393	1/1	0.94	0.39	52,52,52,52	0
56	MG	1A	3463	1/1	0.94	0.50	60,60,60,60	0
56	MG	1A	3522	1/1	0.94	0.23	30,30,30,30	0
56	MG	1A	3120	1/1	0.94	0.17	41,41,41,41	0
56	MG	1a	1805	1/1	0.94	0.14	63,63,63,63	0
56	MG	2A	3139	1/1	0.94	0.37	41,41,41,41	0
56	MG	1A	3869	1/1	0.94	0.11	65,65,65,65	0
56	MG	1A	3465	1/1	0.94	0.76	48,48,48,48	0
56	MG	2A	3402	1/1	0.94	0.12	56,56,56,56	0
56	MG	1E	302	1/1	0.94	0.33	27,27,27,27	0
56	MG	2A	3404	1/1	0.94	0.31	41,41,41,41	0
56	MG	1E	303	1/1	0.94	0.37	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3146	1/1	0.94	0.28	59,59,59,59	0
56	MG	2A	3148	1/1	0.94	0.27	51,51,51,51	0
56	MG	2t	201	1/1	0.94	0.06	55,55,55,55	0
56	MG	1a	1813	1/1	0.94	0.09	58,58,58,58	0
56	MG	1A	3871	1/1	0.94	0.29	50,50,50,50	0
56	MG	1A	3872	1/1	0.94	0.35	61,61,61,61	0
56	MG	1A	3206	1/1	0.94	0.18	75,75,75,75	0
56	MG	1A	3467	1/1	0.94	0.14	29,29,29,29	0
56	MG	1A	3468	1/1	0.94	0.40	40,40,40,40	0
56	MG	1a	1828	1/1	0.94	0.11	66,66,66,66	0
56	MG	1A	3614	1/1	0.94	0.47	73,73,73,73	0
57	KAN	1A	3934	33/33	0.94	0.20	39,48,55,63	0
56	MG	1A	3536	1/1	0.94	0.38	38,38,38,38	0
56	MG	1A	3292	1/1	0.94	0.19	36,36,36,36	0
56	MG	2a	1608	1/1	0.94	0.13	61,61,61,61	0
56	MG	2A	3420	1/1	0.94	0.38	52,52,52,52	0
56	MG	1A	3186	1/1	0.94	0.17	68,68,68,68	0
56	MG	1A	3697	1/1	0.94	0.14	55,55,55,55	0
58	ZN	29	501	1/1	0.94	0.08	88,88,88,88	0
58	ZN	2n	501	1/1	0.94	0.06	103,103,103,103	0
56	MG	1A	3177	1/1	0.95	0.20	65,65,65,65	0
56	MG	1A	3043	1/1	0.95	0.26	58,58,58,58	0
56	MG	1A	3453	1/1	0.95	0.34	56,56,56,56	0
56	MG	2A	3339	1/1	0.95	0.26	48,48,48,48	0
56	MG	1A	3589	1/1	0.95	0.48	47,47,47,47	0
56	MG	1A	3847	1/1	0.95	0.25	46,46,46,46	0
56	MG	1A	3362	1/1	0.95	0.46	36,36,36,36	0
56	MG	1A	3054	1/1	0.95	0.32	40,40,40,40	0
56	MG	1A	3047	1/1	0.95	0.22	32,32,32,32	0
56	MG	1A	3258	1/1	0.95	0.34	44,44,44,44	0
56	MG	1a	1866	1/1	0.95	0.14	73,73,73,73	0
56	MG	1A	3259	1/1	0.95	0.33	27,27,27,27	0
56	MG	1A	3854	1/1	0.95	0.13	39,39,39,39	0
56	MG	1A	3516	1/1	0.95	0.41	31,31,31,31	0
56	MG	1A	3517	1/1	0.95	0.42	41,41,41,41	0
56	MG	2A	3141	1/1	0.95	0.20	40,40,40,40	0
56	MG	2A	3354	1/1	0.95	0.09	84,84,84,84	0
56	MG	1A	3009	1/1	0.95	0.09	51,51,51,51	0
56	MG	2a	1681	1/1	0.95	0.08	64,64,64,64	0
56	MG	1x	113	1/1	0.95	0.29	67,67,67,67	0
56	MG	2a	1683	1/1	0.95	0.13	83,83,83,83	0
56	MG	1A	3519	1/1	0.95	0.31	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1a	1629	1/1	0.95	0.22	31,31,31,31	0
56	MG	1A	3603	1/1	0.95	0.21	65,65,65,65	0
56	MG	1A	3070	1/1	0.95	0.14	44,44,44,44	0
56	MG	1A	3315	1/1	0.95	0.44	42,42,42,42	0
56	MG	1A	3607	1/1	0.95	0.21	46,46,46,46	0
56	MG	2A	3152	1/1	0.95	0.18	54,54,54,54	0
56	MG	2A	3365	1/1	0.95	0.17	51,51,51,51	0
56	MG	1A	3171	1/1	0.95	0.21	61,61,61,61	0
56	MG	2A	3157	1/1	0.95	0.19	74,74,74,74	0
56	MG	1a	1635	1/1	0.95	0.10	56,56,56,56	0
56	MG	1A	3675	1/1	0.95	0.10	52,52,52,52	0
56	MG	1A	3268	1/1	0.95	0.31	29,29,29,29	0
56	MG	2A	3004	1/1	0.95	0.12	42,42,42,42	0
56	MG	2A	3005	1/1	0.95	0.41	48,48,48,48	0
56	MG	2a	1702	1/1	0.95	0.10	84,84,84,84	0
56	MG	1A	3682	1/1	0.95	0.10	41,41,41,41	0
56	MG	2A	3165	1/1	0.95	0.48	77,77,77,77	0
56	MG	1A	3774	1/1	0.95	0.07	83,83,83,83	0
56	MG	2A	3376	1/1	0.95	0.09	60,60,60,60	0
56	MG	2a	1708	1/1	0.95	0.24	80,80,80,80	0
56	MG	1a	1645	1/1	0.95	0.10	71,71,71,71	0
56	MG	1A	3531	1/1	0.95	0.43	34,34,34,34	0
56	MG	1a	1888	1/1	0.95	0.06	75,75,75,75	0
56	MG	1A	3419	1/1	0.95	0.24	55,55,55,55	0
56	MG	1A	3380	1/1	0.95	0.08	67,67,67,67	0
56	MG	2A	3537	1/1	0.95	0.16	63,63,63,63	0
56	MG	1A	3197	1/1	0.95	0.17	37,37,37,37	0
56	MG	1A	3271	1/1	0.95	0.34	33,33,33,33	0
56	MG	2A	3384	1/1	0.95	0.38	42,42,42,42	0
56	MG	1A	3782	1/1	0.95	0.12	76,76,76,76	0
56	MG	2A	3181	1/1	0.95	0.43	50,50,50,50	0
56	MG	1A	3323	1/1	0.95	0.21	49,49,49,49	0
56	MG	1A	3694	1/1	0.95	0.14	39,39,39,39	0
56	MG	2A	3389	1/1	0.95	0.10	51,51,51,51	0
56	MG	1A	3050	1/1	0.95	0.27	43,43,43,43	0
56	MG	1A	3325	1/1	0.95	0.25	41,41,41,41	0
56	MG	2A	3392	1/1	0.95	0.29	57,57,57,57	0
56	MG	1A	3788	1/1	0.95	0.24	53,53,53,53	0
56	MG	1F	302	1/1	0.95	0.37	56,56,56,56	0
56	MG	1a	1667	1/1	0.95	0.18	66,66,66,66	0
56	MG	1A	3474	1/1	0.95	0.14	45,45,45,45	0
56	MG	2A	3196	1/1	0.95	0.31	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1a	1669	1/1	0.95	0.23	68,68,68,68	0
56	MG	1a	1906	1/1	0.95	0.07	54,54,54,54	0
56	MG	2a	1734	1/1	0.95	0.08	59,59,59,59	0
56	MG	2A	3400	1/1	0.95	0.27	60,60,60,60	0
56	MG	2A	3199	1/1	0.95	0.47	38,38,38,38	0
56	MG	2A	3200	1/1	0.95	0.27	46,46,46,46	0
56	MG	2a	1739	1/1	0.95	0.12	79,79,79,79	0
56	MG	1A	3621	1/1	0.95	0.05	78,78,78,78	0
56	MG	1A	3277	1/1	0.95	0.30	43,43,43,43	0
56	MG	1a	1673	1/1	0.95	0.16	68,68,68,68	0
56	MG	1A	3241	1/1	0.95	0.47	36,36,36,36	0
56	MG	2a	1744	1/1	0.95	0.34	68,68,68,68	0
56	MG	1A	3279	1/1	0.95	0.27	45,45,45,45	0
56	MG	1A	3549	1/1	0.95	0.28	26,26,26,26	0
56	MG	2A	3221	1/1	0.95	0.60	35,35,35,35	0
56	MG	1A	3061	1/1	0.95	0.37	72,72,72,72	0
56	MG	2A	3225	1/1	0.95	0.48	41,41,41,41	0
56	MG	2A	3226	1/1	0.95	0.31	52,52,52,52	0
56	MG	2A	3040	1/1	0.95	0.16	43,43,43,43	0
56	MG	1A	3551	1/1	0.95	0.20	28,28,28,28	0
56	MG	1A	3709	1/1	0.95	0.19	15,15,15,15	0
56	MG	2B	208	1/1	0.95	0.09	67,67,67,67	0
56	MG	2A	3234	1/1	0.95	0.43	43,43,43,43	0
56	MG	1A	3333	1/1	0.95	0.53	45,45,45,45	0
56	MG	1A	3431	1/1	0.95	0.23	66,66,66,66	0
56	MG	2B	212	1/1	0.95	0.10	64,64,64,64	0
56	MG	1A	3556	1/1	0.95	0.18	25,25,25,25	0
56	MG	2A	3048	1/1	0.95	0.24	54,54,54,54	0
56	MG	1A	3632	1/1	0.95	0.18	71,71,71,71	0
56	MG	2A	3424	1/1	0.95	0.21	51,51,51,51	0
56	MG	2a	1770	1/1	0.95	0.27	54,54,54,54	0
56	MG	2A	3425	1/1	0.95	0.18	57,57,57,57	0
56	MG	1a	1925	1/1	0.95	0.07	64,64,64,64	0
56	MG	1a	1796	1/1	0.95	0.25	74,74,74,74	0
56	MG	2A	3249	1/1	0.95	0.37	55,55,55,55	0
56	MG	2A	3430	1/1	0.95	0.20	47,47,47,47	0
56	MG	1A	3334	1/1	0.95	0.24	45,45,45,45	0
56	MG	1A	3898	1/1	0.95	0.18	41,41,41,41	0
56	MG	2A	3434	1/1	0.95	0.10	79,79,79,79	0
56	MG	1A	3718	1/1	0.95	0.22	32,32,32,32	0
56	MG	2A	3059	1/1	0.95	0.35	75,75,75,75	0
56	MG	2A	3260	1/1	0.95	0.25	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3719	1/1	0.95	0.09	57,57,57,57	0
56	MG	1A	3201	1/1	0.95	0.51	52,52,52,52	0
56	MG	1A	3075	1/1	0.95	0.14	56,56,56,56	0
56	MG	1A	3221	1/1	0.95	0.35	55,55,55,55	0
56	MG	28	101	1/1	0.95	0.19	47,47,47,47	0
56	MG	28	102	1/1	0.95	0.10	69,69,69,69	0
56	MG	1A	3249	1/1	0.95	0.28	42,42,42,42	0
56	MG	2a	1602	1/1	0.95	0.37	74,74,74,74	0
56	MG	13	102	1/1	0.95	0.23	53,53,53,53	0
56	MG	2A	3073	1/1	0.95	0.22	44,44,44,44	0
56	MG	1A	3724	1/1	0.95	0.20	47,47,47,47	0
56	MG	1A	3437	1/1	0.95	0.43	42,42,42,42	0
56	MG	2A	3284	1/1	0.95	0.29	60,60,60,60	0
56	MG	1A	3489	1/1	0.95	0.12	45,45,45,45	0
56	MG	2A	3079	1/1	0.95	0.09	74,74,74,74	0
56	MG	15	101	1/1	0.95	0.27	51,51,51,51	0
56	MG	1A	3814	1/1	0.95	0.24	73,73,73,73	0
56	MG	1a	1820	1/1	0.95	0.16	47,47,47,47	0
56	MG	1a	1821	1/1	0.95	0.08	88,88,88,88	0
56	MG	2A	3457	1/1	0.95	0.17	44,44,44,44	0
56	MG	1A	3342	1/1	0.95	0.30	51,51,51,51	0
56	MG	1a	1825	1/1	0.95	0.25	76,76,76,76	0
56	MG	2A	3293	1/1	0.95	0.47	60,60,60,60	0
56	MG	1a	1826	1/1	0.95	0.24	74,74,74,74	0
56	MG	1A	3729	1/1	0.95	0.21	41,41,41,41	0
56	MG	17	101	1/1	0.95	0.16	54,54,54,54	0
56	MG	2A	3298	1/1	0.95	0.53	50,50,50,50	0
56	MG	1a	1951	1/1	0.95	0.06	64,64,64,64	0
56	MG	1A	3294	1/1	0.95	0.36	40,40,40,40	0
56	MG	1A	3819	1/1	0.95	0.24	47,47,47,47	0
56	MG	2a	1819	1/1	0.95	0.54	57,57,57,57	0
56	MG	2a	1628	1/1	0.95	0.08	69,69,69,69	0
56	MG	1A	3731	1/1	0.95	0.18	56,56,56,56	0
56	MG	1A	3440	1/1	0.95	0.27	54,54,54,54	0
56	MG	1A	3222	1/1	0.95	0.47	19,19,19,19	0
56	MG	2a	1824	1/1	0.95	0.09	73,73,73,73	0
56	MG	2a	1633	1/1	0.95	0.13	55,55,55,55	0
56	MG	1A	3573	1/1	0.95	0.07	57,57,57,57	0
56	MG	1a	1839	1/1	0.95	0.25	75,75,75,75	0
56	MG	2e	201	1/1	0.95	0.08	74,74,74,74	0
56	MG	1A	3345	1/1	0.95	0.31	36,36,36,36	0
56	MG	2A	3311	1/1	0.95	0.27	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3203	1/1	0.95	0.14	70,70,70,70	0
56	MG	2A	3314	1/1	0.95	0.37	67,67,67,67	0
56	MG	1A	3062	1/1	0.95	0.35	53,53,53,53	0
56	MG	1A	3498	1/1	0.95	0.20	45,45,45,45	0
56	MG	2x	101	1/1	0.95	0.44	58,58,58,58	0
56	MG	2A	3319	1/1	0.95	0.24	44,44,44,44	0
56	MG	1A	3300	1/1	0.95	0.22	43,43,43,43	0
56	MG	1m	202	1/1	0.95	0.32	58,58,58,58	0
56	MG	2A	3482	1/1	0.95	0.15	60,60,60,60	0
56	MG	1a	1845	1/1	0.95	0.31	54,54,54,54	0
56	MG	2a	1652	1/1	0.95	0.17	76,76,76,76	0
56	MG	2A	3116	1/1	0.95	0.49	42,42,42,42	0
56	MG	2A	3486	1/1	0.95	0.23	54,54,54,54	0
56	MG	1a	1846	1/1	0.95	0.13	42,42,42,42	0
56	MG	1A	3650	1/1	0.95	0.14	56,56,56,56	0
56	MG	1A	3447	1/1	0.95	0.18	53,53,53,53	0
56	MG	1A	3028	1/1	0.95	0.16	57,57,57,57	0
56	MG	1a	1852	1/1	0.95	0.14	72,72,72,72	0
56	MG	1A	3450	1/1	0.95	0.10	47,47,47,47	0
56	MG	1x	122	1/1	0.96	0.15	63,63,63,63	0
56	MG	1A	3329	1/1	0.96	0.16	47,47,47,47	0
56	MG	2A	3156	1/1	0.96	0.26	47,47,47,47	0
56	MG	2a	1675	1/1	0.96	0.07	94,94,94,94	0
56	MG	1a	1639	1/1	0.96	0.26	35,35,35,35	0
56	MG	1A	3095	1/1	0.96	0.42	32,32,32,32	0
56	MG	2A	3002	1/1	0.96	0.34	55,55,55,55	0
56	MG	1A	3469	1/1	0.96	0.08	37,37,37,37	0
56	MG	1A	3876	1/1	0.96	0.12	59,59,59,59	0
56	MG	1A	3524	1/1	0.96	0.48	44,44,44,44	0
56	MG	1A	3332	1/1	0.96	0.47	45,45,45,45	0
56	MG	2A	3164	1/1	0.96	0.34	42,42,42,42	0
56	MG	1A	3594	1/1	0.96	0.26	47,47,47,47	0
56	MG	2A	3166	1/1	0.96	0.23	44,44,44,44	0
56	MG	1A	3528	1/1	0.96	0.53	35,35,35,35	0
56	MG	1A	3114	1/1	0.96	0.30	33,33,33,33	0
56	MG	1A	3654	1/1	0.96	0.10	76,76,76,76	0
56	MG	2a	1689	1/1	0.96	0.28	72,72,72,72	0
56	MG	1A	3297	1/1	0.96	0.34	63,63,63,63	0
56	MG	1a	1771	1/1	0.96	0.12	63,63,63,63	0
56	MG	1A	3157	1/1	0.96	0.36	62,62,62,62	0
56	MG	2A	3173	1/1	0.96	0.42	39,39,39,39	0
56	MG	1A	3030	1/1	0.96	0.15	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	1696	1/1	0.96	0.19	52,52,52,52	0
56	MG	1A	3534	1/1	0.96	0.49	32,32,32,32	0
56	MG	1a	1894	1/1	0.96	0.11	67,67,67,67	0
56	MG	2A	3180	1/1	0.96	0.42	30,30,30,30	0
56	MG	1N	201	1/1	0.96	0.13	66,66,66,66	0
56	MG	1A	3602	1/1	0.96	0.10	48,48,48,48	0
56	MG	1A	3889	1/1	0.96	0.25	61,61,61,61	0
56	MG	1a	1898	1/1	0.96	0.16	78,78,78,78	0
56	MG	2A	3188	1/1	0.96	0.49	30,30,30,30	0
56	MG	1A	3732	1/1	0.96	0.08	68,68,68,68	0
56	MG	1A	3733	1/1	0.96	0.21	32,32,32,32	0
56	MG	1A	3052	1/1	0.96	0.14	26,26,26,26	0
56	MG	2A	3193	1/1	0.96	0.14	51,51,51,51	0
56	MG	1A	3810	1/1	0.96	0.20	65,65,65,65	0
56	MG	1A	3735	1/1	0.96	0.17	37,37,37,37	0
56	MG	1a	1672	1/1	0.96	0.45	60,60,60,60	0
56	MG	1R	201	1/1	0.96	0.21	27,27,27,27	0
56	MG	1A	3736	1/1	0.96	0.19	48,48,48,48	0
56	MG	1a	1675	1/1	0.96	0.20	68,68,68,68	0
56	MG	1A	3896	1/1	0.96	0.12	65,65,65,65	0
56	MG	1a	1911	1/1	0.96	0.13	64,64,64,64	0
56	MG	2A	3205	1/1	0.96	0.49	49,49,49,49	0
56	MG	2A	3206	1/1	0.96	0.45	31,31,31,31	0
56	MG	1a	1677	1/1	0.96	0.25	56,56,56,56	0
56	MG	2a	1721	1/1	0.96	0.17	82,82,82,82	0
56	MG	1A	3738	1/1	0.96	0.12	63,63,63,63	0
56	MG	2A	3211	1/1	0.96	0.49	42,42,42,42	0
56	MG	1A	3477	1/1	0.96	0.40	44,44,44,44	0
56	MG	2A	3214	1/1	0.96	0.56	41,41,41,41	0
56	MG	2A	3216	1/1	0.96	0.49	38,38,38,38	0
56	MG	1A	3662	1/1	0.96	0.43	60,60,60,60	0
56	MG	1A	3816	1/1	0.96	0.25	42,42,42,42	0
56	MG	2A	3559	1/1	0.96	0.08	66,66,66,66	0
56	MG	1A	3605	1/1	0.96	0.08	72,72,72,72	0
56	MG	2A	3045	1/1	0.96	0.27	41,41,41,41	0
56	MG	2A	3406	1/1	0.96	0.16	57,57,57,57	0
56	MG	1A	3071	1/1	0.96	0.35	37,37,37,37	0
56	MG	1a	1685	1/1	0.96	0.06	79,79,79,79	0
56	MG	2a	1735	1/1	0.96	0.05	71,71,71,71	0
56	MG	1Y	201	1/1	0.96	0.11	64,64,64,64	0
56	MG	1A	3099	1/1	0.96	0.20	44,44,44,44	0
56	MG	2A	3230	1/1	0.96	0.44	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3236	1/1	0.96	0.22	48,48,48,48	0
56	MG	1a	1801	1/1	0.96	0.06	53,53,53,53	0
56	MG	2A	3235	1/1	0.96	0.44	47,47,47,47	0
56	MG	1A	3261	1/1	0.96	0.21	25,25,25,25	0
56	MG	1A	3823	1/1	0.96	0.35	50,50,50,50	0
56	MG	1A	3072	1/1	0.96	0.39	45,45,45,45	0
56	MG	2A	3060	1/1	0.96	0.12	48,48,48,48	0
56	MG	1A	3483	1/1	0.96	0.20	48,48,48,48	0
56	MG	1A	3238	1/1	0.96	0.41	28,28,28,28	0
56	MG	1a	1696	1/1	0.96	0.44	46,46,46,46	0
56	MG	2A	3247	1/1	0.96	0.53	41,41,41,41	0
56	MG	2D	301	1/1	0.96	0.29	34,34,34,34	0
56	MG	2a	1752	1/1	0.96	0.23	57,57,57,57	0
56	MG	2a	1753	1/1	0.96	0.37	46,46,46,46	0
56	MG	1A	3827	1/1	0.96	0.26	39,39,39,39	0
56	MG	2a	1755	1/1	0.96	0.69	63,63,63,63	0
56	MG	1A	3829	1/1	0.96	0.24	44,44,44,44	0
56	MG	2A	3068	1/1	0.96	0.36	44,44,44,44	0
56	MG	2A	3427	1/1	0.96	0.16	67,67,67,67	0
56	MG	1A	3309	1/1	0.96	0.38	42,42,42,42	0
56	MG	2A	3072	1/1	0.96	0.14	64,64,64,64	0
56	MG	2A	3259	1/1	0.96	0.17	42,42,42,42	0
56	MG	1A	3349	1/1	0.96	0.38	26,26,26,26	0
56	MG	2a	1765	1/1	0.96	0.24	59,59,59,59	0
56	MG	1A	3046	1/1	0.96	0.38	46,46,46,46	0
56	MG	1a	1819	1/1	0.96	0.20	70,70,70,70	0
56	MG	1a	1704	1/1	0.96	0.47	33,33,33,33	0
56	MG	2A	3266	1/1	0.96	0.29	39,39,39,39	0
56	MG	2A	3077	1/1	0.96	0.29	46,46,46,46	0
56	MG	2A	3438	1/1	0.96	0.18	63,63,63,63	0
56	MG	1a	1705	1/1	0.96	0.23	54,54,54,54	0
56	MG	1a	1822	1/1	0.96	0.13	55,55,55,55	0
56	MG	2A	3273	1/1	0.96	0.64	54,54,54,54	0
56	MG	2A	3275	1/1	0.96	0.51	33,33,33,33	0
56	MG	2A	3443	1/1	0.96	0.17	70,70,70,70	0
56	MG	1A	3084	1/1	0.96	0.19	54,54,54,54	0
56	MG	1A	3553	1/1	0.96	0.26	34,34,34,34	0
56	MG	1a	1945	1/1	0.96	0.23	61,61,61,61	0
56	MG	1a	1708	1/1	0.96	0.54	49,49,49,49	0
56	MG	1a	1827	1/1	0.96	0.31	68,68,68,68	0
56	MG	1A	3921	1/1	0.96	0.35	43,43,43,43	0
56	MG	1a	1949	1/1	0.96	0.49	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1a	1829	1/1	0.96	0.22	70,70,70,70	0
56	MG	18	104	1/1	0.96	0.66	52,52,52,52	0
56	MG	1A	3676	1/1	0.96	0.16	57,57,57,57	0
56	MG	2a	1791	1/1	0.96	0.13	68,68,68,68	0
56	MG	1A	3840	1/1	0.96	0.20	71,71,71,71	0
56	MG	19	103	1/1	0.96	0.07	63,63,63,63	0
56	MG	2A	3097	1/1	0.96	0.26	48,48,48,48	0
56	MG	1A	3677	1/1	0.96	0.13	56,56,56,56	0
56	MG	1A	3038	1/1	0.96	0.12	26,26,26,26	0
56	MG	1a	1837	1/1	0.96	0.37	44,44,44,44	0
56	MG	1A	3359	1/1	0.96	0.14	32,32,32,32	0
56	MG	2A	3299	1/1	0.96	0.33	64,64,64,64	0
56	MG	1A	3360	1/1	0.96	0.26	29,29,29,29	0
56	MG	1A	3684	1/1	0.96	0.25	53,53,53,53	0
56	MG	1A	3243	1/1	0.96	0.10	51,51,51,51	0
56	MG	1a	1721	1/1	0.96	0.17	81,81,81,81	0
56	MG	2a	1622	1/1	0.96	0.15	92,92,92,92	0
56	MG	2a	1805	1/1	0.96	0.31	95,95,95,95	0
56	MG	2A	3111	1/1	0.96	0.30	29,29,29,29	0
56	MG	1A	3276	1/1	0.96	0.25	52,52,52,52	0
56	MG	1A	3405	1/1	0.96	0.17	60,60,60,60	0
56	MG	2a	1627	1/1	0.96	0.20	78,78,78,78	0
56	MG	2a	1810	1/1	0.96	0.18	67,67,67,67	0
56	MG	1A	3448	1/1	0.96	0.42	42,42,42,42	0
56	MG	1A	3317	1/1	0.96	0.22	55,55,55,55	0
56	MG	2A	3309	1/1	0.96	0.46	53,53,53,53	0
56	MG	1A	3407	1/1	0.96	0.10	85,85,85,85	0
56	MG	1A	3695	1/1	0.96	0.17	55,55,55,55	0
56	MG	1a	1849	1/1	0.96	0.30	61,61,61,61	0
56	MG	1r	101	1/1	0.96	0.14	64,64,64,64	0
56	MG	1A	3696	1/1	0.96	0.11	49,49,49,49	0
56	MG	1a	1851	1/1	0.96	0.06	64,64,64,64	0
56	MG	2A	3320	1/1	0.96	0.18	42,42,42,42	0
56	MG	2a	1641	1/1	0.96	0.12	62,62,62,62	0
56	MG	1A	3182	1/1	0.96	0.17	53,53,53,53	0
56	MG	2A	3323	1/1	0.96	0.27	40,40,40,40	0
56	MG	2a	1645	1/1	0.96	0.21	56,56,56,56	0
56	MG	1A	3365	1/1	0.96	0.47	20,20,20,20	0
56	MG	1A	3245	1/1	0.96	0.20	40,40,40,40	0
56	MG	1B	210	1/1	0.96	0.38	35,35,35,35	0
56	MG	2A	3485	1/1	0.96	0.22	58,58,58,58	0
56	MG	1A	3367	1/1	0.96	0.14	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3369	1/1	0.96	0.38	43,43,43,43	0
56	MG	1a	1621	1/1	0.96	0.30	39,39,39,39	0
56	MG	1A	3220	1/1	0.96	0.15	38,38,38,38	0
56	MG	1A	3040	1/1	0.96	0.15	49,49,49,49	0
56	MG	1A	3705	1/1	0.96	0.14	50,50,50,50	0
56	MG	2A	3334	1/1	0.96	0.20	62,62,62,62	0
56	MG	1A	3372	1/1	0.96	0.34	36,36,36,36	0
56	MG	1a	1865	1/1	0.96	0.09	59,59,59,59	0
56	MG	1A	3373	1/1	0.96	0.39	52,52,52,52	0
56	MG	2x	105	1/1	0.96	0.46	61,61,61,61	0
56	MG	1A	3286	1/1	0.96	0.34	23,23,23,23	0
56	MG	1A	3375	1/1	0.96	0.37	25,25,25,25	0
56	MG	1A	3022	1/1	0.96	0.40	57,57,57,57	0
57	KAN	1A	3935	33/33	0.96	0.18	27,36,51,59	0
57	KAN	1a	1955	33/33	0.96	0.19	44,52,58,59	0
56	MG	1A	3077	1/1	0.96	0.08	69,69,69,69	0
56	MG	1A	3712	1/1	0.96	0.16	37,37,37,37	0
56	MG	1x	117	1/1	0.96	0.18	57,57,57,57	0
56	MG	2A	3147	1/1	0.96	0.56	65,65,65,65	0
56	MG	1A	3059	1/1	0.96	0.11	30,30,30,30	0
56	MG	1A	3714	1/1	0.96	0.18	34,34,34,34	0
58	ZN	26	102	1/1	0.96	0.13	63,63,63,63	0
56	MG	1A	3112	1/1	0.96	0.41	23,23,23,23	0
56	MG	1a	1637	1/1	0.96	0.20	54,54,54,54	0
56	MG	2A	3347	1/1	0.97	0.43	42,42,42,42	0
56	MG	1A	3156	1/1	0.97	0.04	59,59,59,59	0
56	MG	1a	1910	1/1	0.97	0.16	52,52,52,52	0
56	MG	1A	3690	1/1	0.97	0.15	33,33,33,33	0
56	MG	2A	3351	1/1	0.97	0.13	58,58,58,58	0
56	MG	1a	1802	1/1	0.97	0.11	52,52,52,52	0
56	MG	1a	1803	1/1	0.97	0.23	59,59,59,59	0
56	MG	2A	3174	1/1	0.97	0.27	48,48,48,48	0
56	MG	2A	3031	1/1	0.97	0.41	47,47,47,47	0
56	MG	2A	3177	1/1	0.97	0.37	47,47,47,47	0
56	MG	1a	1914	1/1	0.97	0.09	74,74,74,74	0
56	MG	1A	3925	1/1	0.97	0.20	48,48,48,48	0
56	MG	1A	3560	1/1	0.97	0.47	36,36,36,36	0
56	MG	1a	1806	1/1	0.97	0.19	62,62,62,62	0
56	MG	2a	1692	1/1	0.97	0.13	67,67,67,67	0
56	MG	1a	1919	1/1	0.97	0.09	57,57,57,57	0
56	MG	1A	3093	1/1	0.97	0.38	21,21,21,21	0
56	MG	2A	3185	1/1	0.97	0.46	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3186	1/1	0.97	0.51	38,38,38,38	0
56	MG	1a	1602	1/1	0.97	0.52	67,67,67,67	0
56	MG	1A	3381	1/1	0.97	0.08	59,59,59,59	0
56	MG	1A	3505	1/1	0.97	0.10	46,46,46,46	0
56	MG	1A	3048	1/1	0.97	0.39	46,46,46,46	0
56	MG	1A	3462	1/1	0.97	0.06	59,59,59,59	0
56	MG	1A	3767	1/1	0.97	0.13	34,34,34,34	0
56	MG	1A	3566	1/1	0.97	0.43	34,34,34,34	0
56	MG	2a	1704	1/1	0.97	0.16	69,69,69,69	0
56	MG	2A	3046	1/1	0.97	0.14	76,76,76,76	0
56	MG	1a	1710	1/1	0.97	0.43	43,43,43,43	0
56	MG	1B	202	1/1	0.97	0.25	55,55,55,55	0
56	MG	2A	3050	1/1	0.97	0.26	53,53,53,53	0
56	MG	2A	3052	1/1	0.97	0.21	57,57,57,57	0
56	MG	1A	3122	1/1	0.97	0.39	40,40,40,40	0
56	MG	1A	3699	1/1	0.97	0.06	51,51,51,51	0
56	MG	2A	3204	1/1	0.97	0.36	38,38,38,38	0
56	MG	1A	3239	1/1	0.97	0.35	23,23,23,23	0
56	MG	1a	1823	1/1	0.97	0.05	69,69,69,69	0
56	MG	1A	3569	1/1	0.97	0.47	34,34,34,34	0
56	MG	2A	3208	1/1	0.97	0.41	42,42,42,42	0
56	MG	1A	3571	1/1	0.97	0.45	30,30,30,30	0
56	MG	1A	3262	1/1	0.97	0.17	32,32,32,32	0
56	MG	1a	1937	1/1	0.97	0.27	52,52,52,52	0
56	MG	1A	3086	1/1	0.97	0.06	30,30,30,30	0
56	MG	2A	3215	1/1	0.97	0.52	35,35,35,35	0
56	MG	2A	3062	1/1	0.97	0.22	59,59,59,59	0
56	MG	1A	3776	1/1	0.97	0.10	43,43,43,43	0
56	MG	1A	3574	1/1	0.97	0.28	18,18,18,18	0
56	MG	1A	3044	1/1	0.97	0.30	34,34,34,34	0
56	MG	2A	3222	1/1	0.97	0.32	49,49,49,49	0
56	MG	1A	3779	1/1	0.97	0.07	71,71,71,71	0
56	MG	2A	3224	1/1	0.97	0.24	45,45,45,45	0
56	MG	1A	3514	1/1	0.97	0.28	34,34,34,34	0
56	MG	2A	3070	1/1	0.97	0.42	61,61,61,61	0
56	MG	1a	1833	1/1	0.97	0.14	59,59,59,59	0
56	MG	2A	3228	1/1	0.97	0.32	28,28,28,28	0
56	MG	1A	3267	1/1	0.97	0.31	40,40,40,40	0
56	MG	1A	3305	1/1	0.97	0.26	53,53,53,53	0
56	MG	1A	3108	1/1	0.97	0.41	27,27,27,27	0
56	MG	2A	3232	1/1	0.97	0.15	46,46,46,46	0
56	MG	1A	3307	1/1	0.97	0.30	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3520	1/1	0.97	0.34	17,17,17,17	0
56	MG	2A	3236	1/1	0.97	0.46	33,33,33,33	0
56	MG	1A	3786	1/1	0.97	0.19	51,51,51,51	0
56	MG	2B	205	1/1	0.97	0.06	91,91,91,91	0
56	MG	1A	3472	1/1	0.97	0.08	60,60,60,60	0
56	MG	1A	3144	1/1	0.97	0.23	72,72,72,72	0
56	MG	1A	3715	1/1	0.97	0.11	68,68,68,68	0
56	MG	2A	3241	1/1	0.97	0.55	39,39,39,39	0
56	MG	1A	3523	1/1	0.97	0.14	43,43,43,43	0
56	MG	1A	3350	1/1	0.97	0.26	30,30,30,30	0
56	MG	2A	3415	1/1	0.97	0.39	43,43,43,43	0
56	MG	1A	3352	1/1	0.97	0.36	32,32,32,32	0
56	MG	2A	3246	1/1	0.97	0.47	31,31,31,31	0
56	MG	2a	1751	1/1	0.97	0.19	62,62,62,62	0
56	MG	1A	3526	1/1	0.97	0.34	28,28,28,28	0
56	MG	2A	3248	1/1	0.97	0.34	57,57,57,57	0
56	MG	1a	1636	1/1	0.97	0.12	55,55,55,55	0
56	MG	2A	3250	1/1	0.97	0.20	57,57,57,57	0
56	MG	2a	1756	1/1	0.97	0.24	68,68,68,68	0
56	MG	2a	1757	1/1	0.97	0.27	57,57,57,57	0
56	MG	1A	3527	1/1	0.97	0.50	25,25,25,25	0
56	MG	2A	3252	1/1	0.97	0.23	59,59,59,59	0
56	MG	1A	3200	1/1	0.97	0.20	66,66,66,66	0
56	MG	1A	3593	1/1	0.97	0.36	55,55,55,55	0
56	MG	1A	3355	1/1	0.97	0.26	23,23,23,23	0
56	MG	2A	3256	1/1	0.97	0.41	24,24,24,24	0
56	MG	2A	3257	1/1	0.97	0.19	37,37,37,37	0
56	MG	2A	3093	1/1	0.97	0.12	69,69,69,69	0
56	MG	1A	3530	1/1	0.97	0.57	43,43,43,43	0
56	MG	1a	1643	1/1	0.97	0.08	51,51,51,51	0
56	MG	2A	3432	1/1	0.97	0.26	44,44,44,44	0
56	MG	2A	3262	1/1	0.97	0.20	65,65,65,65	0
56	MG	1A	3596	1/1	0.97	0.40	25,25,25,25	0
56	MG	1a	1748	1/1	0.97	0.26	59,59,59,59	0
56	MG	2a	1772	1/1	0.97	0.36	52,52,52,52	0
56	MG	2A	3265	1/1	0.97	0.48	42,42,42,42	0
56	MG	1a	1856	1/1	0.97	0.40	56,56,56,56	0
56	MG	1A	3726	1/1	0.97	0.17	63,63,63,63	0
56	MG	2a	1776	1/1	0.97	0.23	80,80,80,80	0
56	MG	1A	3017	1/1	0.97	0.12	64,64,64,64	0
56	MG	2A	3103	1/1	0.97	0.09	59,59,59,59	0
56	MG	2A	3271	1/1	0.97	0.47	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3106	1/1	0.97	0.28	52,52,52,52	0
56	MG	1A	3273	1/1	0.97	0.45	21,21,21,21	0
56	MG	1a	1752	1/1	0.97	0.34	56,56,56,56	0
56	MG	1a	1861	1/1	0.97	0.27	64,64,64,64	0
56	MG	2A	3278	1/1	0.97	0.33	38,38,38,38	0
56	MG	1a	1648	1/1	0.97	0.15	51,51,51,51	0
56	MG	2A	3281	1/1	0.97	0.41	40,40,40,40	0
56	MG	2A	3449	1/1	0.97	0.21	61,61,61,61	0
56	MG	2A	3282	1/1	0.97	0.38	46,46,46,46	0
56	MG	1A	3274	1/1	0.97	0.23	43,43,43,43	0
56	MG	1A	3314	1/1	0.97	0.42	39,39,39,39	0
56	MG	1A	3246	1/1	0.97	0.24	41,41,41,41	0
56	MG	1A	3090	1/1	0.97	0.19	54,54,54,54	0
56	MG	1A	3111	1/1	0.97	0.48	24,24,24,24	0
56	MG	1a	1658	1/1	0.97	0.48	46,46,46,46	0
56	MG	1x	103	1/1	0.97	0.19	68,68,68,68	0
56	MG	2A	3119	1/1	0.97	0.34	45,45,45,45	0
56	MG	2A	3120	1/1	0.97	0.39	51,51,51,51	0
56	MG	2A	3121	1/1	0.97	0.34	33,33,33,33	0
56	MG	1A	3808	1/1	0.97	0.09	52,52,52,52	0
56	MG	1a	1870	1/1	0.97	0.07	62,62,62,62	0
56	MG	2a	1626	1/1	0.97	0.30	53,53,53,53	0
56	MG	1A	3131	1/1	0.97	0.39	52,52,52,52	0
56	MG	1A	3444	1/1	0.97	0.23	38,38,38,38	0
56	MG	1A	3280	1/1	0.97	0.23	51,51,51,51	0
56	MG	1a	1767	1/1	0.97	0.11	60,60,60,60	0
56	MG	1a	1664	1/1	0.97	0.16	53,53,53,53	0
56	MG	2a	1632	1/1	0.97	0.16	58,58,58,58	0
56	MG	1A	3737	1/1	0.97	0.14	61,61,61,61	0
56	MG	1A	3321	1/1	0.97	0.35	27,27,27,27	0
56	MG	1x	114	1/1	0.97	0.07	86,86,86,86	0
56	MG	1A	3100	1/1	0.97	0.39	25,25,25,25	0
56	MG	1A	3897	1/1	0.97	0.19	51,51,51,51	0
56	MG	2a	1638	1/1	0.97	0.18	59,59,59,59	0
56	MG	1A	3547	1/1	0.97	0.36	42,42,42,42	0
56	MG	2a	1640	1/1	0.97	0.29	64,64,64,64	0
56	MG	1A	3899	1/1	0.97	0.14	53,53,53,53	0
56	MG	1A	3368	1/1	0.97	0.42	24,24,24,24	0
56	MG	2A	3310	1/1	0.97	0.74	56,56,56,56	0
56	MG	1A	3742	1/1	0.97	0.26	41,41,41,41	0
56	MG	2A	3138	1/1	0.97	0.21	65,65,65,65	0
56	MG	1A	3284	1/1	0.97	0.21	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3056	1/1	0.97	0.08	55,55,55,55	0
56	MG	1A	3820	1/1	0.97	0.32	28,28,28,28	0
56	MG	1A	3036	1/1	0.97	0.33	32,32,32,32	0
56	MG	1a	1678	1/1	0.97	0.19	42,42,42,42	0
56	MG	1A	3289	1/1	0.97	0.25	35,35,35,35	0
56	MG	2a	1653	1/1	0.97	0.21	49,49,49,49	0
56	MG	2A	3145	1/1	0.97	0.05	66,66,66,66	0
56	MG	1A	3115	1/1	0.97	0.32	31,31,31,31	0
56	MG	1A	3116	1/1	0.97	0.25	24,24,24,24	0
56	MG	2A	3326	1/1	0.97	0.53	30,30,30,30	0
56	MG	1A	3678	1/1	0.97	0.32	43,43,43,43	0
56	MG	2A	3006	1/1	0.97	0.24	57,57,57,57	0
56	MG	1A	3117	1/1	0.97	0.44	41,41,41,41	0
56	MG	1A	3680	1/1	0.97	0.14	58,58,58,58	0
56	MG	1A	3828	1/1	0.97	0.06	49,49,49,49	0
56	MG	1A	3619	1/1	0.97	0.11	28,28,28,28	0
56	MG	2x	106	1/1	0.97	0.36	54,54,54,54	0
56	MG	2A	3012	1/1	0.97	0.28	33,33,33,33	0
56	MG	1A	3830	1/1	0.97	0.20	42,42,42,42	0
56	MG	2A	3335	1/1	0.97	0.33	42,42,42,42	0
56	MG	1A	3234	1/1	0.97	0.34	25,25,25,25	0
56	MG	1A	3295	1/1	0.97	0.34	39,39,39,39	0
56	MG	1a	1690	1/1	0.97	0.14	53,53,53,53	0
56	MG	1a	1794	1/1	0.97	0.19	40,40,40,40	0
56	MG	1a	1903	1/1	0.97	0.20	61,61,61,61	0
58	ZN	1Y	202	1/1	0.97	0.13	66,66,66,66	0
56	MG	1A	3685	1/1	0.97	0.13	47,47,47,47	0
56	MG	1A	3686	1/1	0.97	0.23	15,15,15,15	0
56	MG	1a	1797	1/1	0.97	0.18	72,72,72,72	0
56	MG	1A	3836	1/1	0.97	0.08	27,27,27,27	0
56	MG	2A	3024	1/1	0.97	0.35	48,48,48,48	0
56	MG	1A	3622	1/1	0.97	0.28	44,44,44,44	0
56	MG	1A	3041	1/1	0.98	0.17	25,25,25,25	0
56	MG	2A	3233	1/1	0.98	0.25	38,38,38,38	0
56	MG	1A	3094	1/1	0.98	0.49	25,25,25,25	0
56	MG	1a	1656	1/1	0.98	0.37	53,53,53,53	0
56	MG	1A	3148	1/1	0.98	0.07	65,65,65,65	0
56	MG	1A	3281	1/1	0.98	0.32	34,34,34,34	0
56	MG	1x	108	1/1	0.98	0.27	42,42,42,42	0
56	MG	1a	1917	1/1	0.98	0.19	62,62,62,62	0
56	MG	1a	1659	1/1	0.98	0.24	40,40,40,40	0
56	MG	1A	3540	1/1	0.98	0.29	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3242	1/1	0.98	0.59	35,35,35,35	0
56	MG	1A	3063	1/1	0.98	0.20	39,39,39,39	0
56	MG	1A	3283	1/1	0.98	0.64	39,39,39,39	0
56	MG	1D	304	1/1	0.98	0.12	57,57,57,57	0
56	MG	1A	3543	1/1	0.98	0.37	26,26,26,26	0
56	MG	2A	3067	1/1	0.98	0.22	80,80,80,80	0
56	MG	1a	1724	1/1	0.98	0.11	75,75,75,75	0
56	MG	2A	3153	1/1	0.98	0.18	69,69,69,69	0
56	MG	2A	3069	1/1	0.98	0.23	45,45,45,45	0
56	MG	2A	3155	1/1	0.98	0.12	60,60,60,60	0
56	MG	1a	1665	1/1	0.98	0.14	43,43,43,43	0
56	MG	1A	3916	1/1	0.98	0.14	63,63,63,63	0
56	MG	1A	3618	1/1	0.98	0.29	58,58,58,58	0
56	MG	2A	3358	1/1	0.98	0.16	60,60,60,60	0
56	MG	1a	1728	1/1	0.98	0.04	77,77,77,77	0
56	MG	1A	3580	1/1	0.98	0.40	35,35,35,35	0
56	MG	2A	3566	1/1	0.98	0.28	43,43,43,43	0
56	MG	1A	3581	1/1	0.98	0.51	24,24,24,24	0
56	MG	2A	3258	1/1	0.98	0.50	43,43,43,43	0
56	MG	1A	3544	1/1	0.98	0.25	16,16,16,16	0
56	MG	1A	3104	1/1	0.98	0.39	39,39,39,39	0
56	MG	2a	1780	1/1	0.98	0.32	56,56,56,56	0
56	MG	2A	3078	1/1	0.98	0.27	35,35,35,35	0
56	MG	1A	3584	1/1	0.98	0.26	28,28,28,28	0
56	MG	2A	3001	1/1	0.98	0.23	88,88,88,88	0
56	MG	2A	3081	1/1	0.98	0.14	59,59,59,59	0
56	MG	1A	3546	1/1	0.98	0.53	33,33,33,33	0
56	MG	1a	1735	1/1	0.98	0.23	80,80,80,80	0
56	MG	2A	3084	1/1	0.98	0.29	43,43,43,43	0
56	MG	2a	1788	1/1	0.98	0.14	62,62,62,62	0
56	MG	1A	3831	1/1	0.98	0.11	54,54,54,54	0
56	MG	2A	3269	1/1	0.98	0.29	35,35,35,35	0
56	MG	1A	3747	1/1	0.98	0.19	66,66,66,66	0
56	MG	1A	3264	1/1	0.98	0.29	32,32,32,32	0
56	MG	2A	3272	1/1	0.98	0.12	58,58,58,58	0
56	MG	1A	3126	1/1	0.98	0.12	74,74,74,74	0
56	MG	2A	3274	1/1	0.98	0.55	32,32,32,32	0
56	MG	1A	3335	1/1	0.98	0.47	27,27,27,27	0
56	MG	2A	3009	1/1	0.98	0.06	59,59,59,59	0
56	MG	1A	3288	1/1	0.98	0.17	32,32,32,32	0
56	MG	2F	303	1/1	0.98	0.24	65,65,65,65	0
56	MG	1Q	201	1/1	0.98	0.13	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3279	1/1	0.98	0.46	31,31,31,31	0
56	MG	1A	3311	1/1	0.98	0.23	42,42,42,42	0
56	MG	1A	3088	1/1	0.98	0.13	43,43,43,43	0
56	MG	2A	3095	1/1	0.98	0.27	41,41,41,41	0
56	MG	1a	1810	1/1	0.98	0.10	63,63,63,63	0
56	MG	2A	3184	1/1	0.98	0.10	54,54,54,54	0
56	MG	1A	3839	1/1	0.98	0.13	58,58,58,58	0
56	MG	1A	3339	1/1	0.98	0.29	26,26,26,26	0
56	MG	1A	3340	1/1	0.98	0.29	36,36,36,36	0
56	MG	1A	3055	1/1	0.98	0.18	41,41,41,41	0
56	MG	1A	3888	1/1	0.98	0.17	68,68,68,68	0
56	MG	1a	1817	1/1	0.98	0.08	53,53,53,53	0
56	MG	2A	3104	1/1	0.98	0.22	45,45,45,45	0
56	MG	2A	3105	1/1	0.98	0.43	56,56,56,56	0
56	MG	1a	1884	1/1	0.98	0.04	70,70,70,70	0
56	MG	1A	3291	1/1	0.98	0.29	31,31,31,31	0
56	MG	1A	3065	1/1	0.98	0.20	22,22,22,22	0
56	MG	2A	3297	1/1	0.98	0.31	41,41,41,41	0
56	MG	1A	3270	1/1	0.98	0.26	31,31,31,31	0
56	MG	1A	3376	1/1	0.98	0.08	75,75,75,75	0
56	MG	1A	3039	1/1	0.98	0.21	50,50,50,50	0
56	MG	2A	3112	1/1	0.98	0.20	42,42,42,42	0
56	MG	2A	3201	1/1	0.98	0.41	35,35,35,35	0
56	MG	2A	3202	1/1	0.98	0.33	38,38,38,38	0
56	MG	1A	3848	1/1	0.98	0.17	43,43,43,43	0
56	MG	1a	1756	1/1	0.98	0.11	55,55,55,55	0
56	MG	1a	1694	1/1	0.98	0.34	46,46,46,46	0
56	MG	1A	3118	1/1	0.98	0.15	37,37,37,37	0
56	MG	1A	3224	1/1	0.98	0.38	23,23,23,23	0
56	MG	13	101	1/1	0.98	0.39	26,26,26,26	0
56	MG	1A	3681	1/1	0.98	0.08	57,57,57,57	0
56	MG	2A	3035	1/1	0.98	0.27	53,53,53,53	0
56	MG	1A	3320	1/1	0.98	0.52	26,26,26,26	0
56	MG	2A	3518	1/1	0.98	0.16	59,59,59,59	0
56	MG	2A	3313	1/1	0.98	0.35	28,28,28,28	0
56	MG	1a	1700	1/1	0.98	0.21	73,73,73,73	0
56	MG	1A	3119	1/1	0.98	0.44	44,44,44,44	0
56	MG	2A	3316	1/1	0.98	0.58	27,27,27,27	0
56	MG	1a	1766	1/1	0.98	0.06	63,63,63,63	0
56	MG	2A	3318	1/1	0.98	0.40	39,39,39,39	0
56	MG	2A	3217	1/1	0.98	0.61	38,38,38,38	0
56	MG	1A	3351	1/1	0.98	0.49	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3219	1/1	0.98	0.58	35,35,35,35	0
56	MG	1a	1703	1/1	0.98	0.26	51,51,51,51	0
56	MG	1A	3275	1/1	0.98	0.53	39,39,39,39	0
56	MG	1A	3902	1/1	0.98	0.14	38,38,38,38	0
56	MG	1A	3034	1/1	0.98	0.22	32,32,32,32	0
56	MG	1A	3687	1/1	0.98	0.13	33,33,33,33	0
56	MG	1A	3211	1/1	0.98	0.37	31,31,31,31	0
56	MG	1B	222	1/1	0.98	0.19	59,59,59,59	0
58	ZN	16	102	1/1	0.98	0.19	48,48,48,48	0
58	ZN	1n	501	1/1	0.98	0.14	64,64,64,64	0
56	MG	1a	1650	1/1	0.98	0.24	38,38,38,38	0
56	MG	1A	3570	1/1	0.98	0.48	25,25,25,25	0
58	ZN	25	501	1/1	0.98	0.17	66,66,66,66	0
56	MG	2A	3051	1/1	0.98	0.24	47,47,47,47	0
56	MG	1x	101	1/1	0.98	0.09	75,75,75,75	0
56	MG	1A	3503	1/1	0.98	0.35	36,36,36,36	0
56	MG	1A	3506	1/1	0.99	0.27	43,43,43,43	0
56	MG	2A	3209	1/1	0.99	0.47	35,35,35,35	0
56	MG	1A	3266	1/1	0.99	0.37	26,26,26,26	0
56	MG	1a	1759	1/1	0.99	0.13	62,62,62,62	0
56	MG	2A	3212	1/1	0.99	0.56	43,43,43,43	0
56	MG	1A	3495	1/1	0.99	0.09	47,47,47,47	0
56	MG	1a	1655	1/1	0.99	0.16	56,56,56,56	0
56	MG	1A	3285	1/1	0.99	0.28	26,26,26,26	0
56	MG	2a	1643	1/1	0.99	0.24	59,59,59,59	0
56	MG	1A	3214	1/1	0.99	0.31	55,55,55,55	0
56	MG	1A	3354	1/1	0.99	0.47	25,25,25,25	0
56	MG	2A	3189	1/1	0.99	0.24	55,55,55,55	0
56	MG	1A	3045	1/1	0.99	0.23	37,37,37,37	0
56	MG	1A	3555	1/1	0.99	0.23	42,42,42,42	0
56	MG	1A	3346	1/1	0.99	0.29	44,44,44,44	0
56	MG	1a	1812	1/1	0.99	0.31	54,54,54,54	0
56	MG	1A	3357	1/1	0.99	0.59	31,31,31,31	0
56	MG	1a	1642	1/1	0.99	0.11	68,68,68,68	0
56	MG	2A	3283	1/1	0.99	0.42	50,50,50,50	0
56	MG	1a	1624	1/1	0.99	0.06	59,59,59,59	0
56	MG	1A	3515	1/1	0.99	0.31	30,30,30,30	0
56	MG	2A	3021	1/1	0.99	0.18	48,48,48,48	0
56	MG	1A	3330	1/1	0.99	0.40	25,25,25,25	0
56	MG	1A	3228	1/1	0.99	0.40	33,33,33,33	0
58	ZN	15	104	1/1	0.99	0.15	49,49,49,49	0
56	MG	1A	3037	1/1	0.99	0.23	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	ZN	19	104	1/1	0.99	0.18	52,52,52,52	0
56	MG	2A	3049	1/1	0.99	0.09	79,79,79,79	0
56	MG	2A	3321	1/1	0.99	0.60	54,54,54,54	0
56	MG	2A	3176	1/1	0.99	0.39	41,41,41,41	0
56	MG	1B	224	1/1	0.99	0.09	39,39,39,39	0
56	MG	1a	1649	1/1	0.99	0.26	42,42,42,42	0
56	MG	1A	3652	1/1	0.99	0.28	43,43,43,43	0
56	MG	1A	3123	1/1	0.99	0.26	26,26,26,26	0
59	SF4	1d	303	8/8	0.99	0.17	60,65,69,72	0
59	SF4	2d	501	8/8	0.99	0.15	60,79,85,85	0
56	MG	2A	3100	1/1	1.00	0.36	37,37,37,37	0

6.5 Other polymers (i)

There are no such residues in this entry.