Full wwPDB X-ray Structure Validation Report ⓘ

Nov 6, 2023 – 06:03 PM EST

PDB ID	:	6OF1
Title	:	Crystal structure of the Thermus thermophilus 70S ribosome in complex with dirithromycin and bound to mRNA and A-, P-, and E-site tRNAs at 2.80A resolution
Authors	:	Khabibullina, N.F.; Tereshchenkov, A.G.; Komarova, E.S.; Syroegin, E.A.; Shiriaev, D.I.; Paleskava, A.; Kartsev, V.G.; Bogdanov, A.A.; Konevega, A.L.; Dontsova, O.A.; Sergiev, P.V.; Osterman, I.A.; Polikanov, Y.S.
Deposited on	:	2019-03-28
Resolution	:	2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The 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:

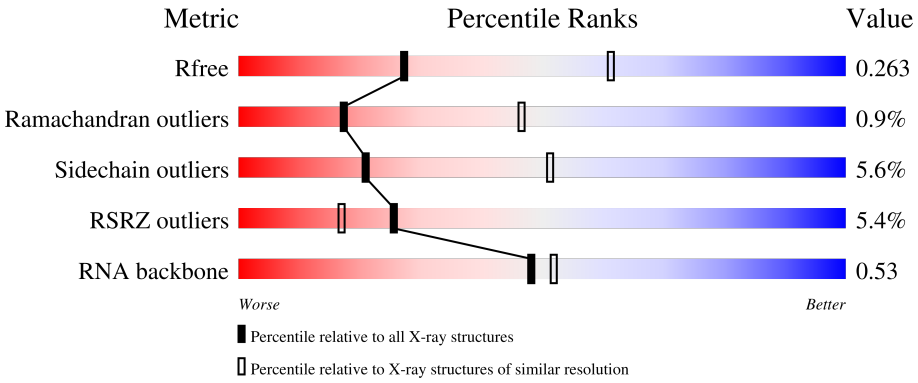
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

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 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)
RNA backbone	3102	1227 (3.10-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	% 79% 16%
2	1B	121	91% 7%

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

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Mol	Chain	Length	Quality of chain
2	2B	121	88% 11%
3	1D	276	94% 6%
3	2D	276	4% 95% 5%
4	1E	206	2% 91% 8%
4	2E	206	6% 95%
5	1F	210	90% 7%
5	2F	210	4% 91% 5%
6	1G	182	93% 7%
6	2G	182	12% 92% 8%
7	1H	180	2% 93%
7	2H	180	15% 91% 6%
8	1I	148	93% 6%
8	2I	148	4% 92% 7%
9	1N	140	94% 6%
9	2N	140	18% 96%
10	1O	122	2% 96%
10	2O	122	7% 94% 6%
11	1P	150	94% 5%
11	2P	150	7% 95%
12	1Q	141	5% 93% 7%
12	2Q	141	12% 95% 5%
13	1R	118	92% 8%
13	2R	118	4% 93% 7%
14	1S	112	2% 94%
14	2S	112	5% 93% 5%

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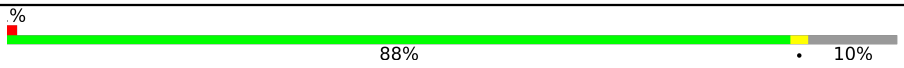
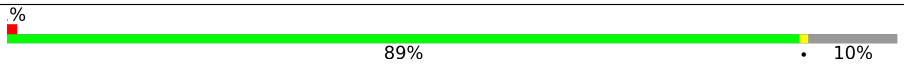
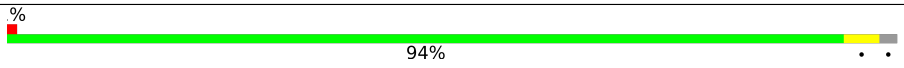
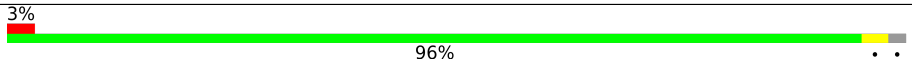
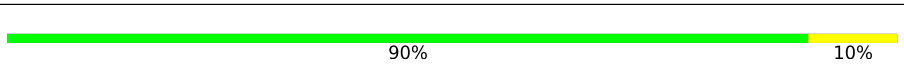
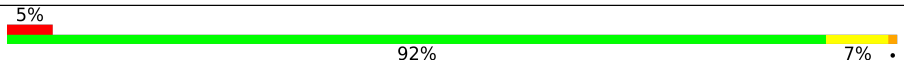
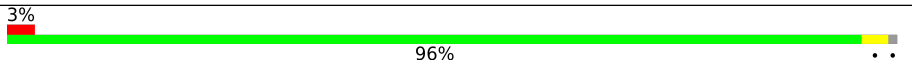
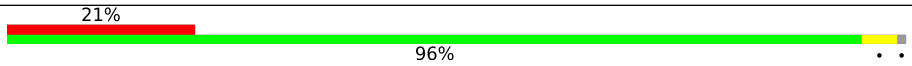
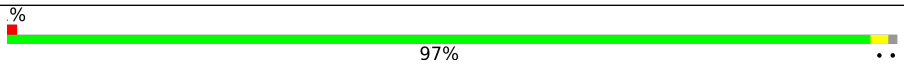
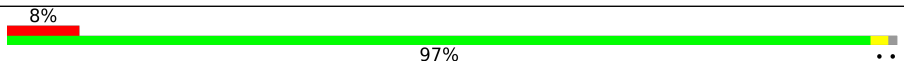
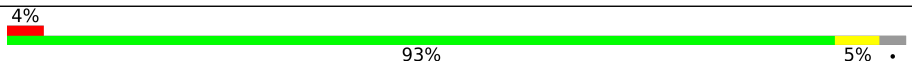
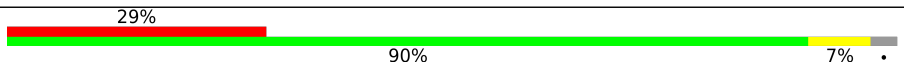
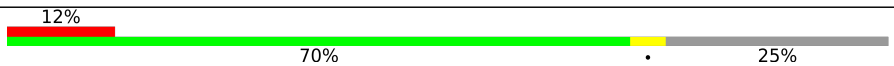
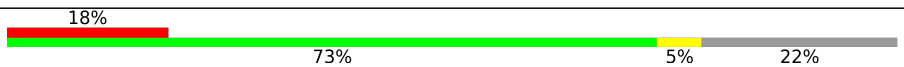
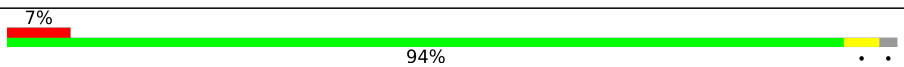
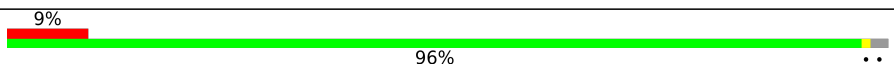
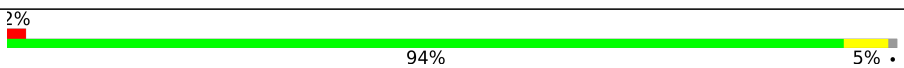
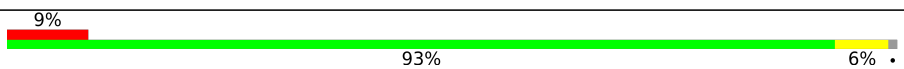
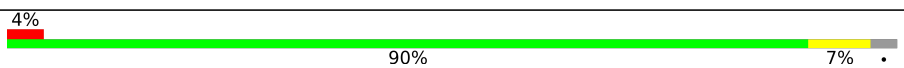
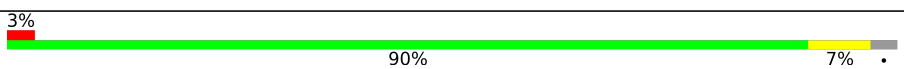
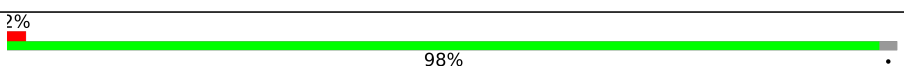
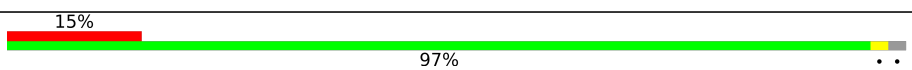
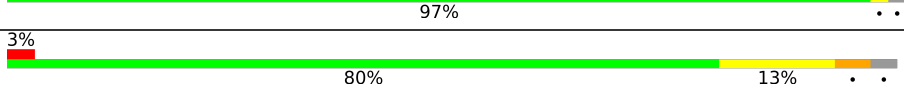
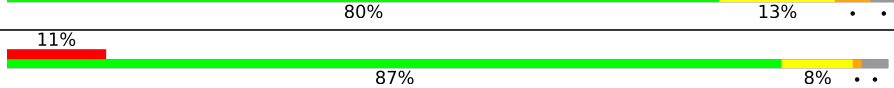
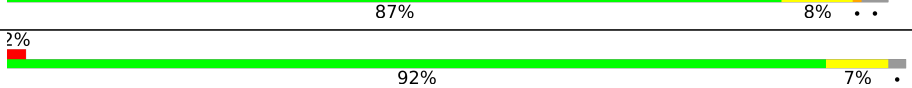
Mol	Chain	Length	Quality of chain
15	1T	146	
15	2T	146	
16	1U	118	
16	2U	118	
17	1V	101	
17	2V	101	
18	1W	113	
18	2W	113	
19	1X	96	
19	2X	96	
20	1Y	110	
20	2Y	110	
21	1Z	206	
21	2Z	206	
22	10	85	
22	20	85	
23	11	98	
23	21	98	
24	12	72	
24	22	72	
25	13	60	
25	23	60	
26	14	71	
26	24	71	
27	15	60	

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Mol	Chain	Length	Quality of chain
27	25	60	2% 90% 8%
28	16	54	4% 89% 9%
28	26	54	7% 93% 6%
29	17	49	10% 92% 6%
29	27	49	18% 94%
30	18	65	88% 11%
30	28	65	15% 89% 9%
31	19	37	3% 97%
31	29	37	27% 97%
32	1a	1521	% 81% 17%
32	2a	1521	% 79% 19%
33	1b	256	3% 84% 7% 10%
33	2b	256	24% 85% 5% 10%
34	1c	239	5% 83% 14%
34	2c	239	18% 82% 14%
35	1d	209	16% 90% 9%
35	2d	209	27% 94% 6%
36	1e	162	7% 85% 6% 9%
36	2e	162	20% 89% 9%
37	1f	101	7% 96%
37	2f	101	95%
38	1g	156	6% 96%
38	2g	156	12% 97%
39	1h	138	4% 92% 7%
39	2h	138	7% 96%

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Mol	Chain	Length	Quality of chain
40	1i	128	8% 96%
40	2i	128	34% 94% 5%
41	1j	105	7% 87% 6% 8%
41	2j	105	23% 86% 6% 9%
42	1k	129	2% 86% 12%
42	2k	129	4% 84% 12%
43	1l	132	3% 86% 7% 8%
43	2l	132	16% 86% 6% 8%
44	1m	126	6% 94%
44	2m	126	18% 92% 5%
45	1n	61	3% 89% 10%
45	2n	61	48% 95%
46	1o	89	2% 97%
46	2o	89	3% 98%
47	1p	88	11% 85% 8% 7%
47	2p	88	13% 86% 7% 7%
48	1q	105	5% 94% 6%
48	2q	105	14% 91% 6%
49	1r	88	% 75% 23%
49	2r	88	77% 23%
50	1s	93	2% 87% 11%
50	2s	93	19% 84% 5% 11%
51	1t	106	7% 84% 6% 9%
51	2t	106	9% 84% 7% 9%
52	1u	27	30% 85% 15%

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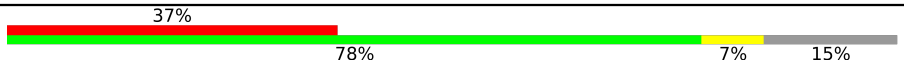
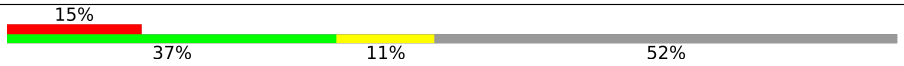
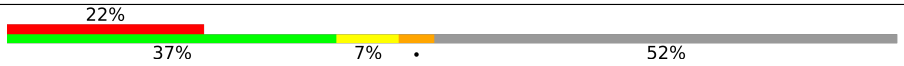
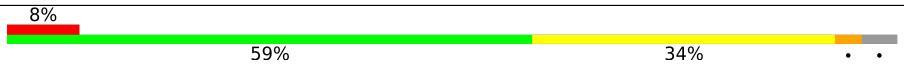
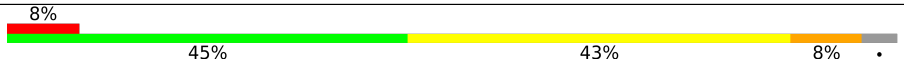
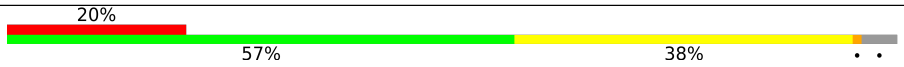
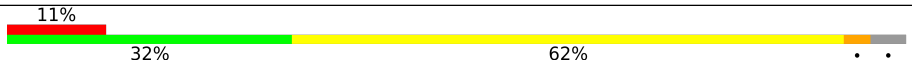
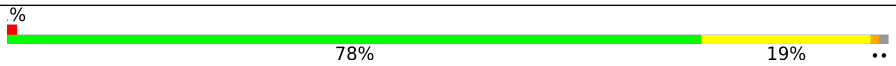
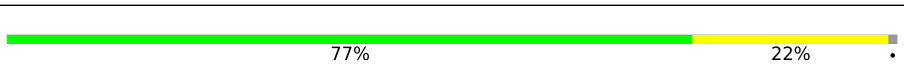
Mol	Chain	Length	Quality of chain
52	2u	27	
53	1v	27	
53	2v	27	
54	1w	76	
54	1y	76	
54	2w	76	
54	2y	76	
55	1x	77	
55	2x	77	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	CM0	2y	34	-	-	-	X
56	MG	15	103	-	-	-	X
56	MG	1A	3017	-	-	-	X
56	MG	1A	3125	-	-	-	X
56	MG	1A	3132	-	-	-	X
56	MG	1A	3133	-	-	-	X
56	MG	1A	3178	-	-	-	X
56	MG	1A	3223	-	-	-	X
56	MG	1A	3224	-	-	-	X
56	MG	1A	3282	-	-	-	X
56	MG	1A	3293	-	-	-	X
56	MG	1A	3366	-	-	-	X
56	MG	1A	3376	-	-	-	X
56	MG	1A	3397	-	-	-	X
56	MG	1A	3425	-	-	-	X
56	MG	1A	3436	-	-	-	X
56	MG	1A	3463	-	-	-	X
56	MG	1A	3489	-	-	-	X
56	MG	1A	3498	-	-	-	X
56	MG	1A	3502	-	-	-	X
56	MG	1A	3518	-	-	-	X
56	MG	1A	3553	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1A	3848	-	-	-	X
56	MG	1A	3911	-	-	-	X
56	MG	1A	3978	-	-	-	X
56	MG	1A	3979	-	-	-	X
56	MG	1A	4081	-	-	-	X
56	MG	1A	4146	-	-	-	X
56	MG	1P	202	-	-	-	X
56	MG	1U	202	-	-	-	X
56	MG	2A	3119	-	-	-	X
56	MG	2A	3285	-	-	-	X
56	MG	2A	3302	-	-	-	X
56	MG	2A	3308	-	-	-	X
56	MG	2A	3312	-	-	-	X
56	MG	2A	3317	-	-	-	X
56	MG	2A	3332	-	-	-	X
56	MG	2A	3352	-	-	-	X
56	MG	2A	3404	-	-	-	X
56	MG	2A	3405	-	-	-	X
56	MG	2A	3411	-	-	-	X
56	MG	2A	3426	-	-	-	X
56	MG	2A	3734	-	-	-	X
56	MG	2A	3781	-	-	-	X
56	MG	2B	203	-	-	-	X
56	MG	2W	202	-	-	-	X
56	MG	2a	1624	-	-	-	X
56	MG	2a	1625	-	-	-	X
56	MG	2a	1627	-	-	-	X
56	MG	2a	1647	-	-	-	X
56	MG	2a	1719	-	-	-	X
56	MG	2a	1804	-	-	-	X

2 Entry composition (i)

There are 61 unique types of molecules in this entry. The entry contains 300274 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 276	C 124	N 48	O 91	P 13	0	0	0
53	2v	13	Total 276	C 124	N 48	O 91	P 13	0	0	0

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
54	1w	73	Total 1568	C 700	N 282	O 512	P 73	S 1	0	0	0
54	1y	73	Total 1568	C 700	N 282	O 512	P 73	S 1	0	0	0
54	2w	73	Total 1568	C 700	N 282	O 512	P 73	S 1	0	0	0
54	2y	73	Total 1568	C 700	N 282	O 512	P 73	S 1	0	0	0

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1A	1148	Total 1148	Mg 1148	0	0
56	2A	860	Total 860	Mg 860	0	0
56	1B	37	Total 37	Mg 37	0	0
56	1D	13	Total 13	Mg 13	0	0
56	1E	8	Total 8	Mg 8	0	0
56	1F	9	Total 9	Mg 9	0	0
56	1G	5	Total 5	Mg 5	0	0
56	1H	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	1I	1	Total Mg 1 1	0	0
56	1N	8	Total Mg 8 8	0	0
56	1O	5	Total Mg 5 5	0	0
56	1P	3	Total Mg 3 3	0	0
56	1Q	6	Total Mg 6 6	0	0
56	1R	2	Total Mg 2 2	0	0
56	1S	3	Total Mg 3 3	0	0
56	1T	2	Total Mg 2 2	0	0
56	1U	7	Total Mg 7 7	0	0
56	1V	2	Total Mg 2 2	0	0
56	1W	6	Total Mg 6 6	0	0
56	1X	5	Total Mg 5 5	0	0
56	1Y	3	Total Mg 3 3	0	0
56	1Z	3	Total Mg 3 3	0	0
56	10	7	Total Mg 7 7	0	0
56	11	4	Total Mg 4 4	0	0
56	12	2	Total Mg 2 2	0	0
56	13	3	Total Mg 3 3	0	0
56	15	5	Total Mg 5 5	0	0
56	16	2	Total Mg 2 2	0	0
56	17	3	Total Mg 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	18	2	Total Mg 2 2	0	0
56	1a	244	Total Mg 244 244	0	0
56	1b	2	Total Mg 2 2	0	0
56	1d	1	Total Mg 1 1	0	0
56	1f	1	Total Mg 1 1	0	0
56	1h	1	Total Mg 1 1	0	0
56	1l	3	Total Mg 3 3	0	0
56	1m	3	Total Mg 3 3	0	0
56	1p	1	Total Mg 1 1	0	0
56	1r	1	Total Mg 1 1	0	0
56	1s	1	Total Mg 1 1	0	0
56	1t	1	Total Mg 1 1	0	0
56	1v	1	Total Mg 1 1	0	0
56	1w	7	Total Mg 7 7	0	0
56	1x	12	Total Mg 12 12	0	0
56	1y	5	Total Mg 5 5	0	0
56	2B	21	Total Mg 21 21	0	0
56	2D	3	Total Mg 3 3	0	0
56	2E	8	Total Mg 8 8	0	0
56	2F	4	Total Mg 4 4	0	0
56	2G	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	2O	2	Total Mg 2 2	0	0
56	2P	3	Total Mg 3 3	0	0
56	2Q	3	Total Mg 3 3	0	0
56	2R	2	Total Mg 2 2	0	0
56	2T	3	Total Mg 3 3	0	0
56	2U	4	Total Mg 4 4	0	0
56	2V	2	Total Mg 2 2	0	0
56	2W	2	Total Mg 2 2	0	0
56	2X	2	Total Mg 2 2	0	0
56	2Z	1	Total Mg 1 1	0	0
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	25	4	Total Mg 4 4	0	0
56	27	1	Total Mg 1 1	0	0
56	28	1	Total Mg 1 1	0	0
56	2a	231	Total Mg 231 231	0	0
56	2d	2	Total Mg 2 2	0	0
56	2e	1	Total Mg 1 1	0	0
56	2f	2	Total Mg 2 2	0	0
56	2g	1	Total Mg 1 1	0	0

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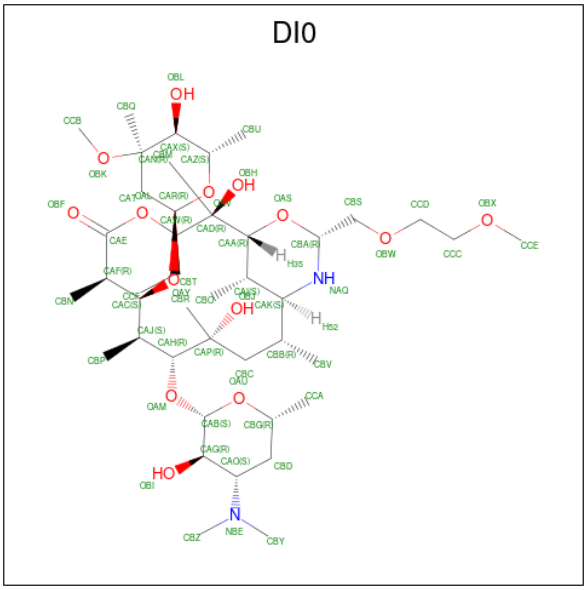
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	2i	1	Total Mg 1 1	0	0
56	2j	2	Total Mg 2 2	0	0
56	2l	2	Total Mg 2 2	0	0
56	2q	3	Total Mg 3 3	0	0
56	2r	1	Total Mg 1 1	0	0
56	2t	1	Total Mg 1 1	0	0
56	2v	3	Total Mg 3 3	0	0
56	2w	1	Total Mg 1 1	0	0
56	2x	5	Total Mg 5 5	0	0
56	2y	7	Total Mg 7 7	0	0

- Molecule 57 is Dirithromycin (three-letter code: DI0) (formula: $C_{42}H_{78}N_2O_{14}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	1A	1	Total C N O 58 42 2 14	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
57	2A	1	Total	C	N	O	0	0
			58	42	2	14		

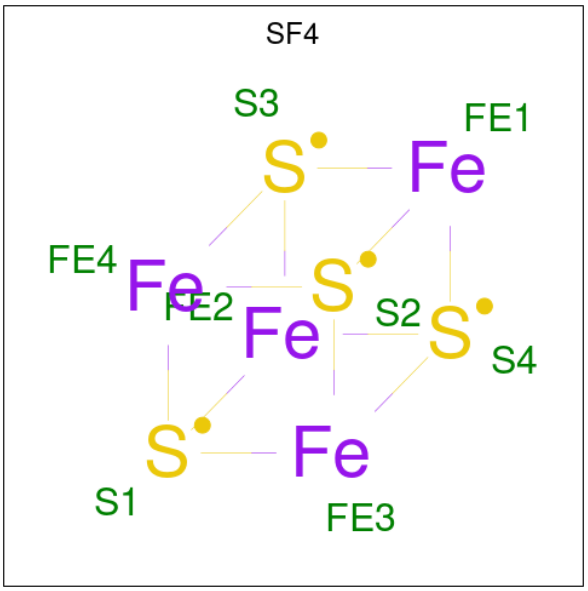
- Molecule 58 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1A	1	Total	K	0	0
			1	1		
58	2A	1	Total	K	0	0
			1	1		

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

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

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



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

- Molecule 61 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1A	2034	Total O 2034 2034	0	0
61	2A	1099	Total O 1099 1099	0	0
61	1B	65	Total O 65 65	0	0
61	1D	29	Total O 29 29	0	0
61	1E	24	Total O 24 24	0	0
61	1F	12	Total O 12 12	0	0
61	1G	5	Total O 5 5	0	0
61	1H	1	Total O 1 1	0	0
61	1I	2	Total O 2 2	0	0
61	1N	6	Total O 6 6	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1O	7	Total O 7 7	0	0
61	1P	23	Total O 23 23	0	0
61	1Q	7	Total O 7 7	0	0
61	1R	14	Total O 14 14	0	0
61	1S	3	Total O 3 3	0	0
61	1T	10	Total O 10 10	0	0
61	1U	12	Total O 12 12	0	0
61	1V	8	Total O 8 8	0	0
61	1W	10	Total O 10 10	0	0
61	1X	4	Total O 4 4	0	0
61	1Y	3	Total O 3 3	0	0
61	10	11	Total O 11 11	0	0
61	11	8	Total O 8 8	0	0
61	12	4	Total O 4 4	0	0
61	13	4	Total O 4 4	0	0
61	15	3	Total O 3 3	0	0
61	16	4	Total O 4 4	0	0
61	17	6	Total O 6 6	0	0
61	18	12	Total O 12 12	0	0
61	19	1	Total O 1 1	0	0
61	1a	439	Total O 439 439	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1b	1	Total O 1 1	0	0
61	1d	2	Total O 2 2	0	0
61	1f	2	Total O 2 2	0	0
61	1g	2	Total O 2 2	0	0
61	1l	11	Total O 11 11	0	0
61	1o	1	Total O 1 1	0	0
61	1p	1	Total O 1 1	0	0
61	1q	2	Total O 2 2	0	0
61	1r	2	Total O 2 2	0	0
61	1t	2	Total O 2 2	0	0
61	1u	1	Total O 1 1	0	0
61	1v	9	Total O 9 9	0	0
61	1w	6	Total O 6 6	0	0
61	1x	7	Total O 7 7	0	0
61	1y	4	Total O 4 4	0	0
61	2B	24	Total O 24 24	0	0
61	2D	20	Total O 20 20	0	0
61	2E	12	Total O 12 12	0	0
61	2F	7	Total O 7 7	0	0
61	2I	4	Total O 4 4	0	0
61	2N	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2O	1	Total O 1 1	0	0
61	2P	12	Total O 12 12	0	0
61	2Q	2	Total O 2 2	0	0
61	2R	2	Total O 2 2	0	0
61	2T	4	Total O 4 4	0	0
61	2U	4	Total O 4 4	0	0
61	2V	1	Total O 1 1	0	0
61	2W	4	Total O 4 4	0	0
61	2X	5	Total O 5 5	0	0
61	2Y	1	Total O 1 1	0	0
61	2Z	1	Total O 1 1	0	0
61	20	3	Total O 3 3	0	0
61	21	6	Total O 6 6	0	0
61	23	2	Total O 2 2	0	0
61	25	1	Total O 1 1	0	0
61	27	3	Total O 3 3	0	0
61	28	4	Total O 4 4	0	0
61	29	1	Total O 1 1	0	0
61	2a	284	Total O 284 284	0	0
61	2d	1	Total O 1 1	0	0
61	2e	2	Total O 2 2	0	0

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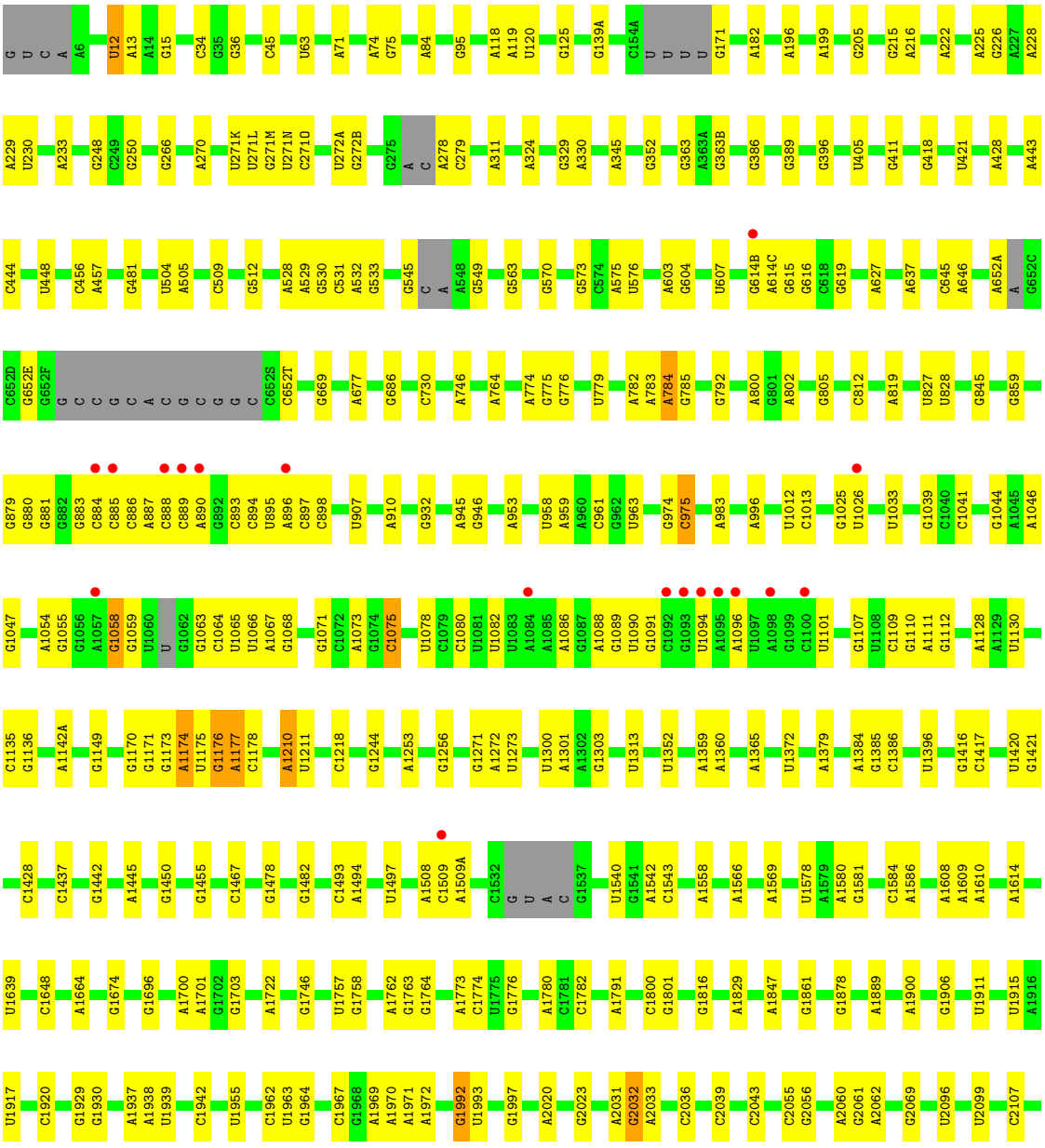
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2g	1	Total O 1 1	0	0
61	2j	3	Total O 3 3	0	0
61	2l	2	Total O 2 2	0	0
61	2n	1	Total O 1 1	0	0
61	2o	1	Total O 1 1	0	0
61	2p	1	Total O 1 1	0	0
61	2q	1	Total O 1 1	0	0
61	2r	1	Total O 1 1	0	0
61	2t	3	Total O 3 3	0	0
61	2v	3	Total O 3 3	0	0
61	2w	3	Total O 3 3	0	0
61	2x	5	Total O 5 5	0	0
61	2y	16	Total O 16 16	0	0

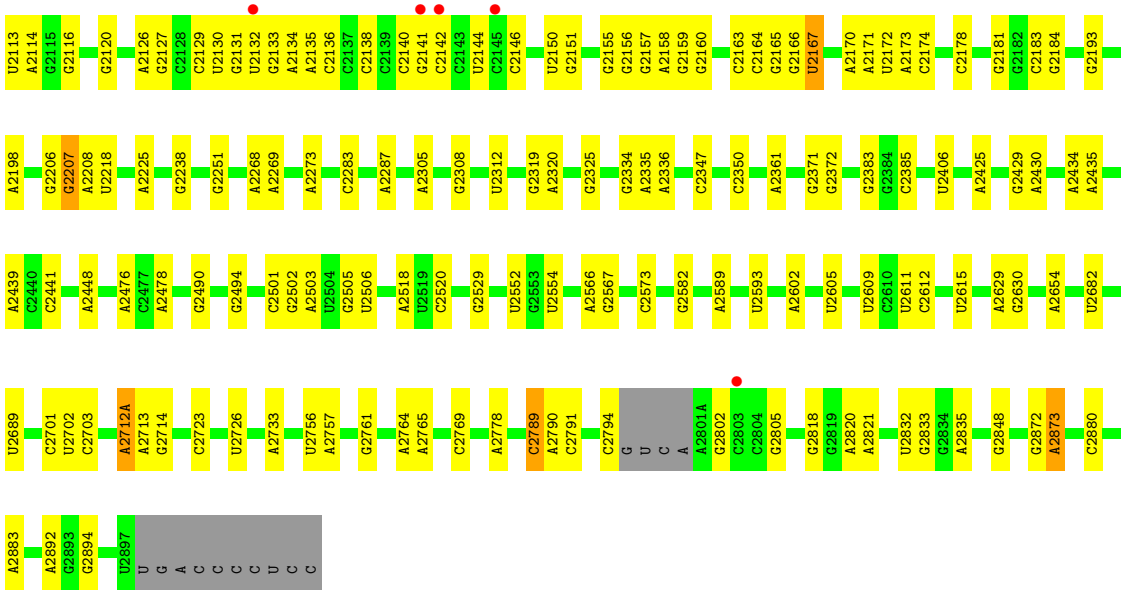
3 Residue-property plots (i)

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

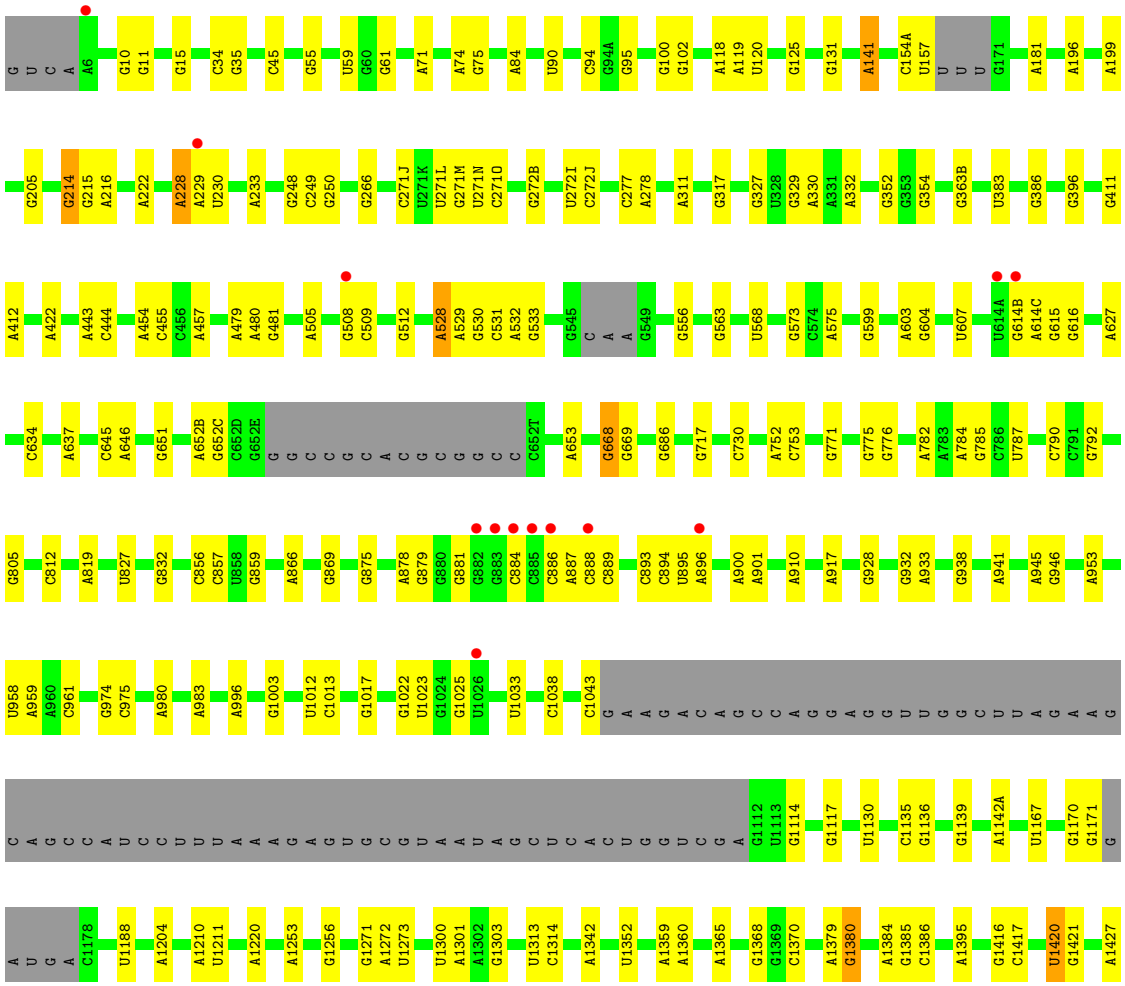
Chain 1A:

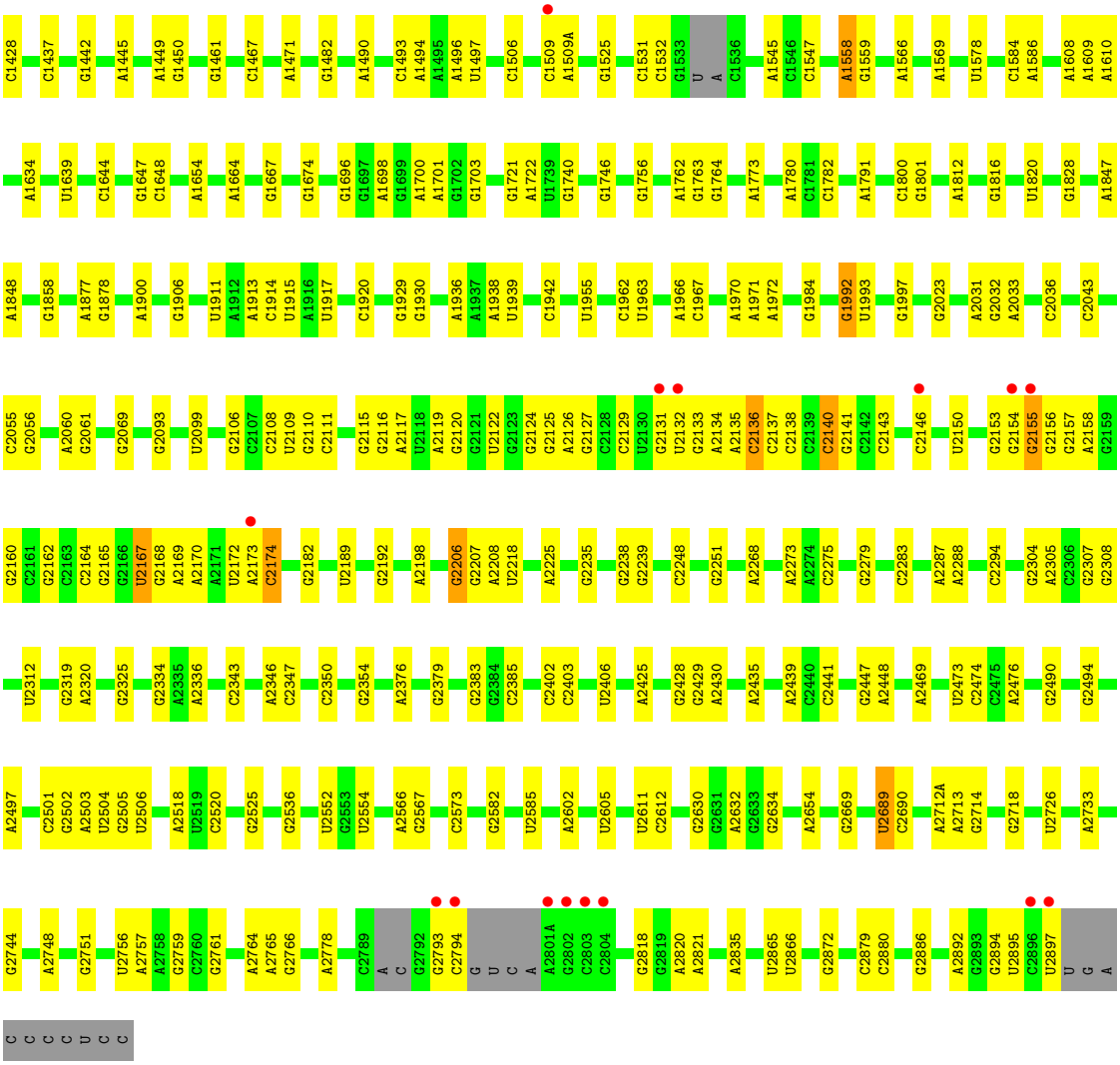




• Molecule 1: 23S Ribosomal RNA

Chain 2A:



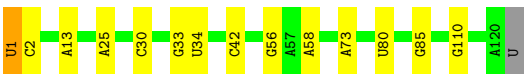


• Molecule 2: 5S Ribosomal RNA

Chain 1B:

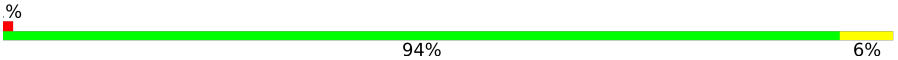
• Molecule 2: 5S Ribosomal RNA

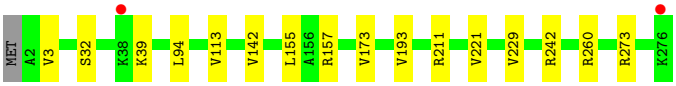
Chain 2B:



• Molecule 3: 50S ribosomal protein L2

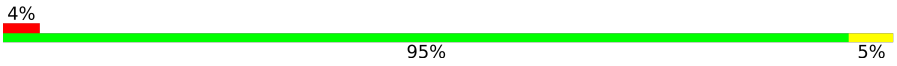
Chain 1D:





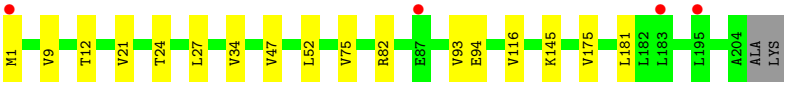
• Molecule 3: 50S ribosomal protein L2

Chain 2D:



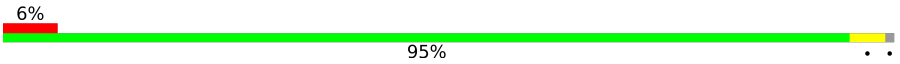
• Molecule 4: 50S ribosomal protein L3

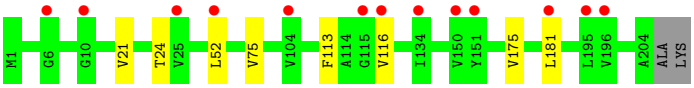
Chain 1E:



• Molecule 4: 50S ribosomal protein L3

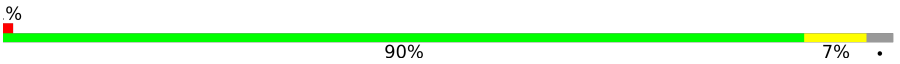
Chain 2E:

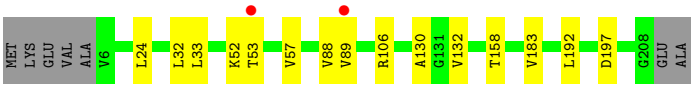




• Molecule 5: 50S ribosomal protein L4

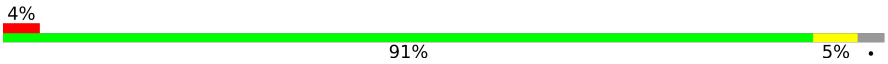
Chain 1F:

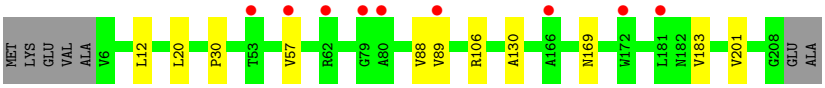




• Molecule 5: 50S ribosomal protein L4

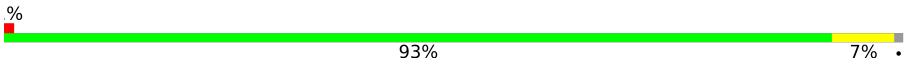
Chain 2F:





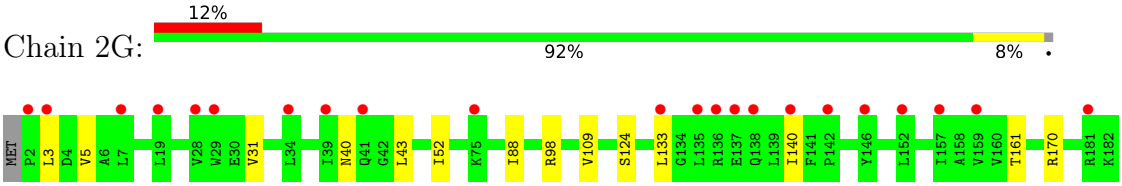
• Molecule 6: 50S ribosomal protein L5

Chain 1G:



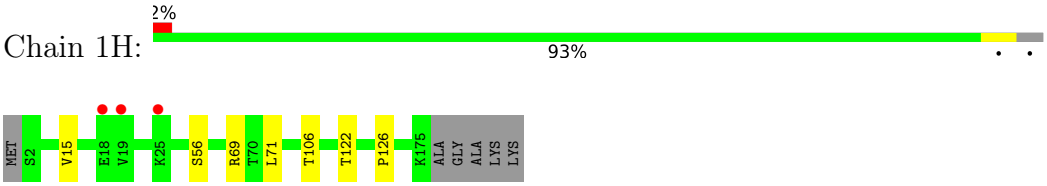
• Molecule 6: 50S ribosomal protein L5

Chain 2G:



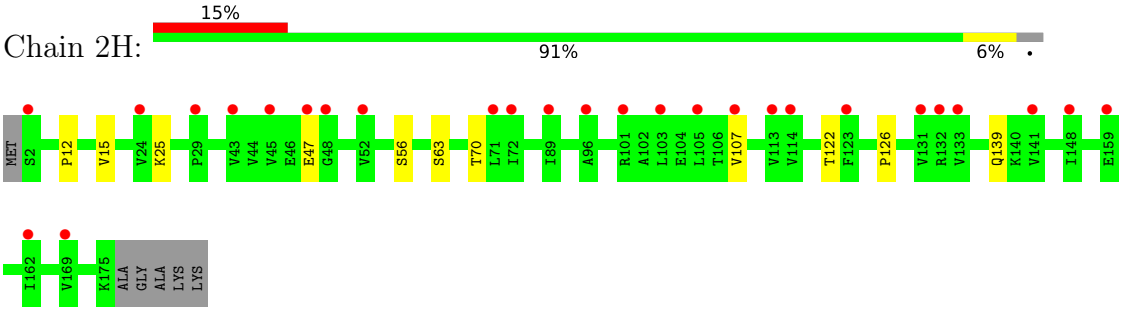
• Molecule 7: 50S ribosomal protein L6

Chain 1H:



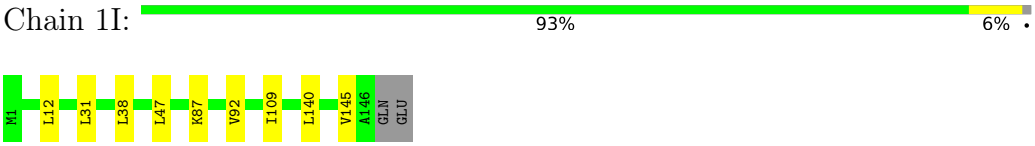
• Molecule 7: 50S ribosomal protein L6

Chain 2H:



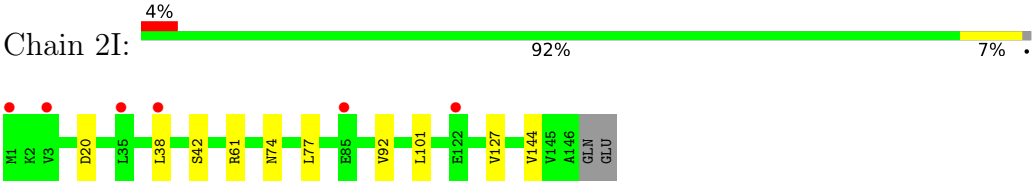
• Molecule 8: 50S ribosomal protein L9

Chain 1I:



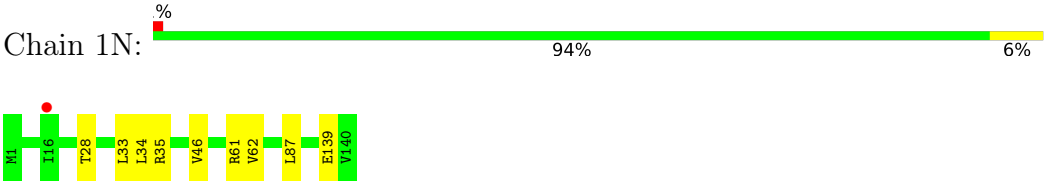
• Molecule 8: 50S ribosomal protein L9

Chain 2I:



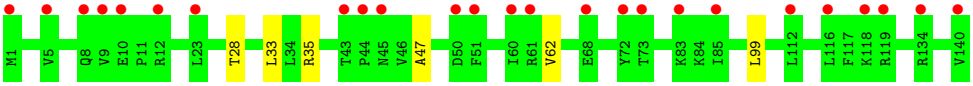
• Molecule 9: 50S ribosomal protein L13

Chain 1N:

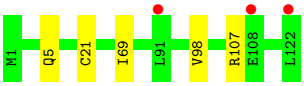


• Molecule 9: 50S ribosomal protein L13

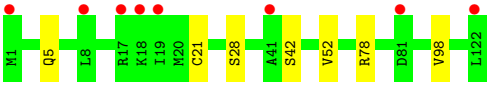
Chain 2N:



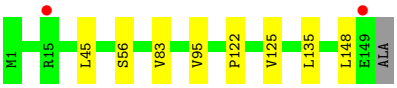
• Molecule 10: 50S ribosomal protein L14



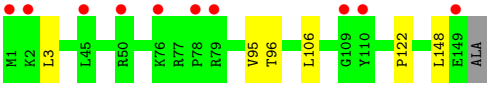
• Molecule 10: 50S ribosomal protein L14



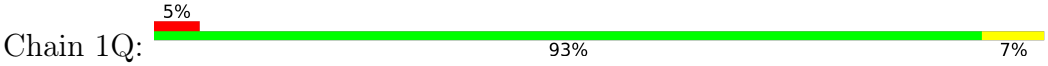
• Molecule 11: 50S ribosomal protein L15

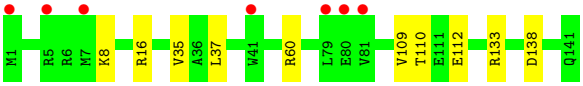


• Molecule 11: 50S ribosomal protein L15

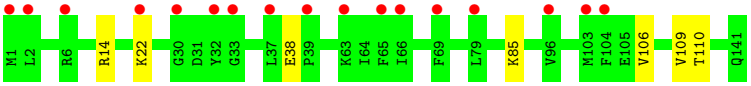


• Molecule 12: 50S ribosomal protein L16



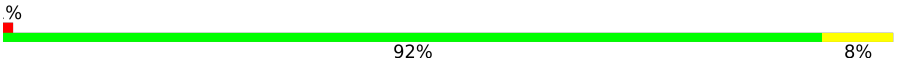


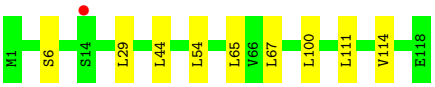
• Molecule 12: 50S ribosomal protein L16



• Molecule 13: 50S ribosomal protein L17

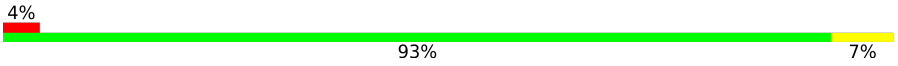
Chain 1R:

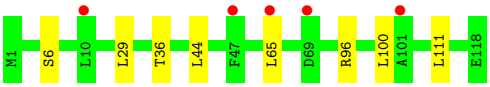




• Molecule 13: 50S ribosomal protein L17

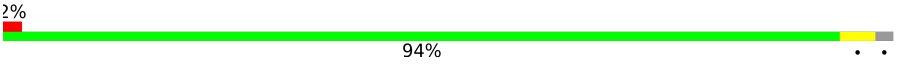
Chain 2R:

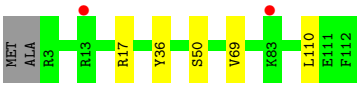




• Molecule 14: 50S ribosomal protein L18

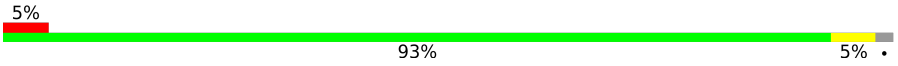
Chain 1S:

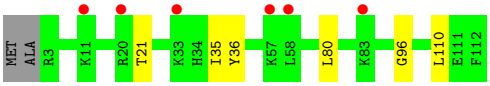




• Molecule 14: 50S ribosomal protein L18

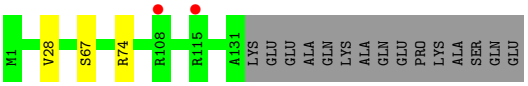
Chain 2S:





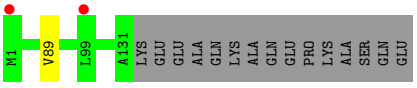
• Molecule 15: 50S ribosomal protein L19

Chain 1T:



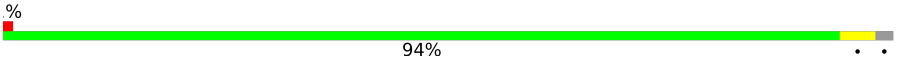
• Molecule 15: 50S ribosomal protein L19

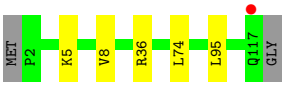
Chain 2T:



• Molecule 16: 50S ribosomal protein L20

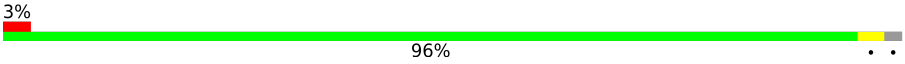
Chain 1U:

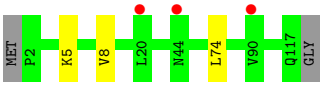




• Molecule 16: 50S ribosomal protein L20

Chain 2U:



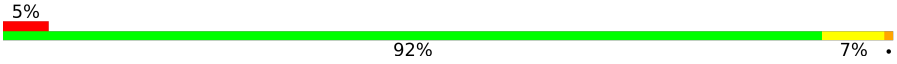


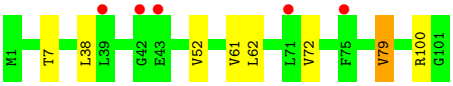
• Molecule 17: 50S ribosomal protein L21

Chain 1V:

• Molecule 17: 50S ribosomal protein L21

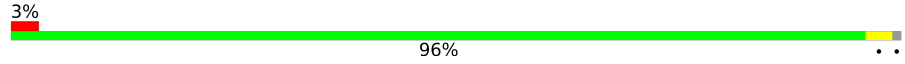
Chain 2V:

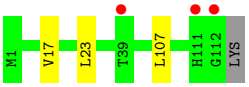




• Molecule 18: 50S ribosomal protein L22

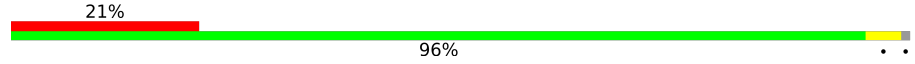
Chain 1W:

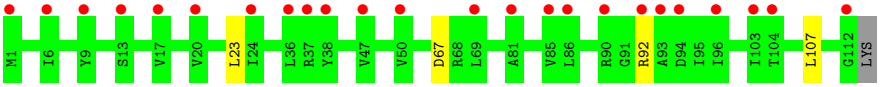




• Molecule 18: 50S ribosomal protein L22

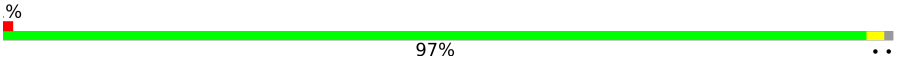
Chain 2W:

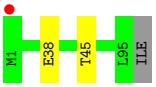




• Molecule 19: 50S ribosomal protein L23

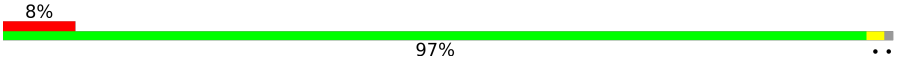
Chain 1X:

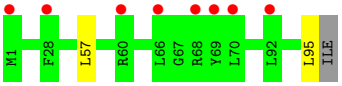




• Molecule 19: 50S ribosomal protein L23

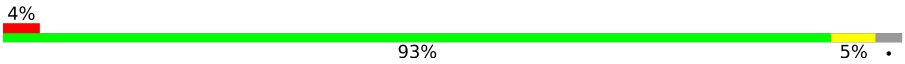
Chain 2X:

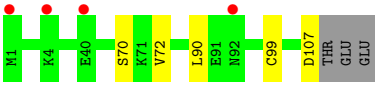




• Molecule 20: 50S ribosomal protein L24

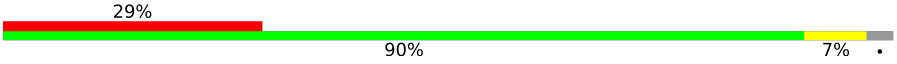
Chain 1Y:

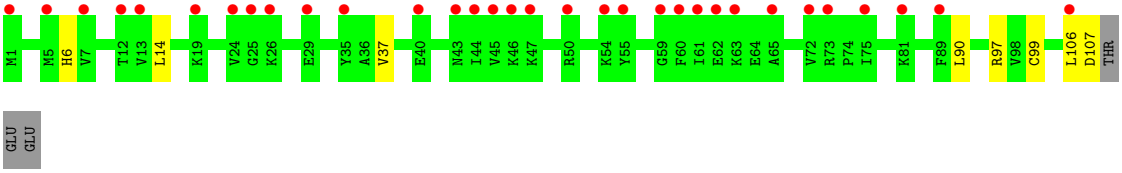




• Molecule 20: 50S ribosomal protein L24

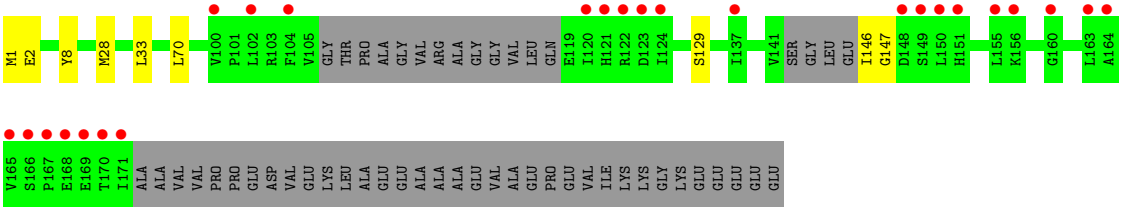
Chain 2Y:





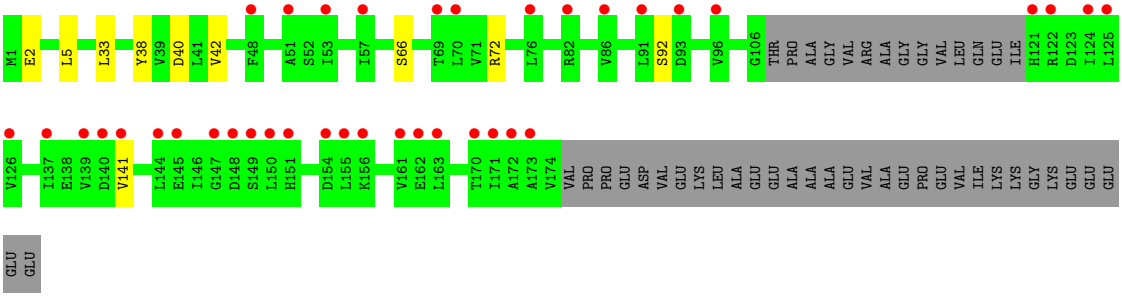
• Molecule 21: 50S ribosomal protein L25

Chain 1Z:



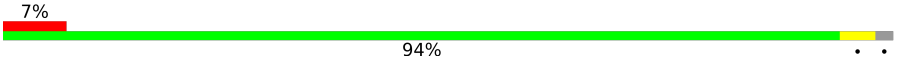
• Molecule 21: 50S ribosomal protein L25

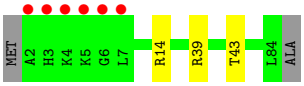
Chain 2Z:



• Molecule 22: 50S ribosomal protein L27

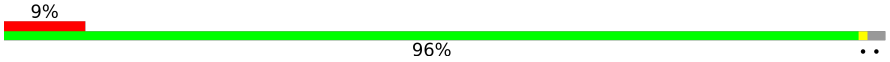
Chain 10:

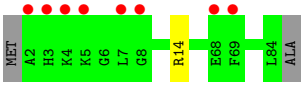




• Molecule 22: 50S ribosomal protein L27

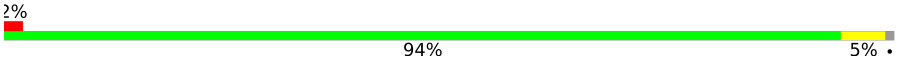
Chain 20:





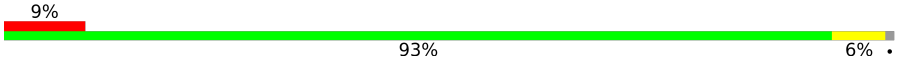
• Molecule 23: 50S ribosomal protein L28

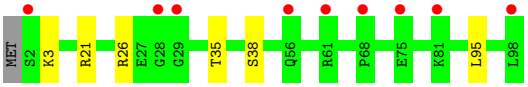
Chain 11:



• Molecule 23: 50S ribosomal protein L28

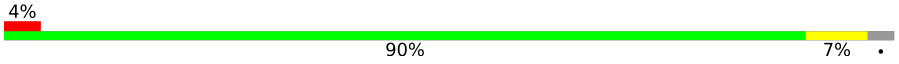
Chain 21:

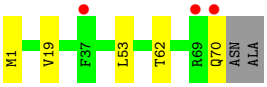




• Molecule 24: 50S ribosomal protein L29

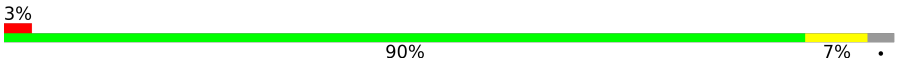
Chain 12:

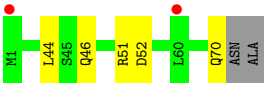




• Molecule 24: 50S ribosomal protein L29

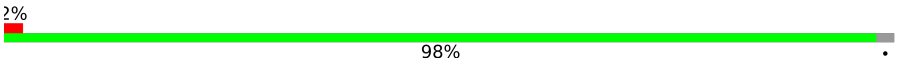
Chain 22:





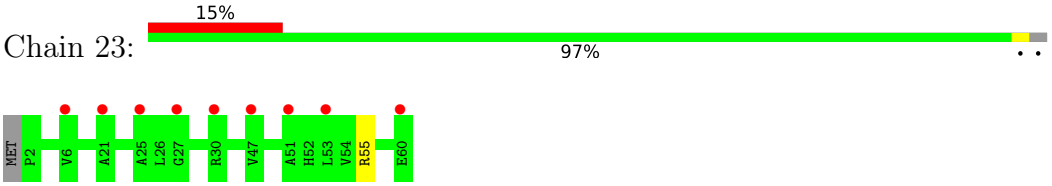
• Molecule 25: 50S ribosomal protein L30

Chain 13:



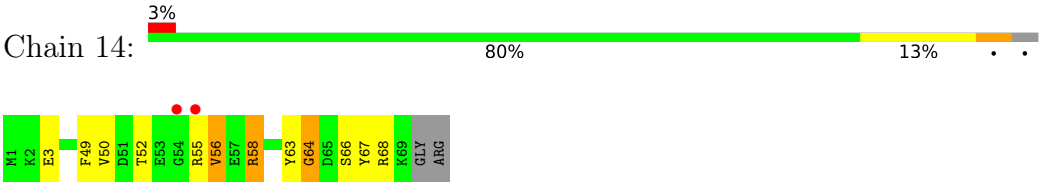
• Molecule 25: 50S ribosomal protein L30

Chain 23:



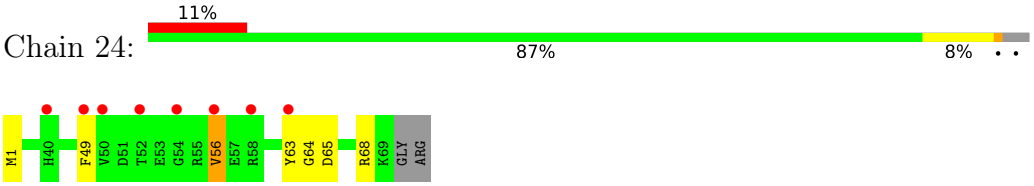
• Molecule 26: 50S ribosomal protein L31

Chain 14:



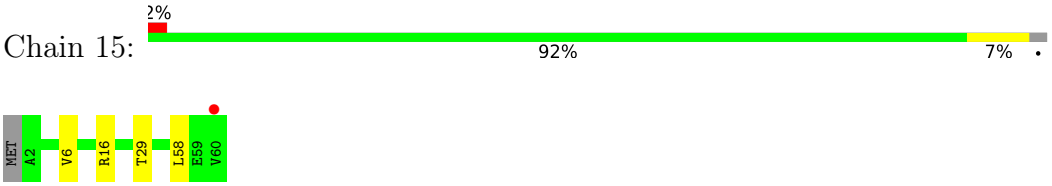
• Molecule 26: 50S ribosomal protein L31

Chain 24:



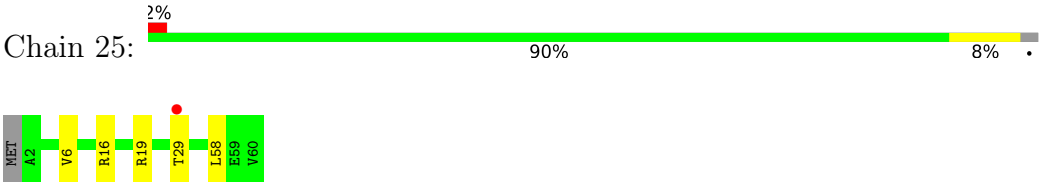
• Molecule 27: 50S ribosomal protein L32

Chain 15:



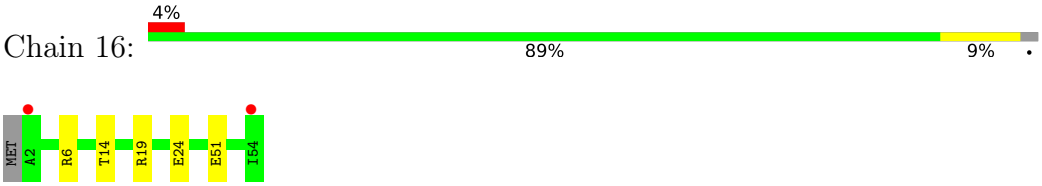
• Molecule 27: 50S ribosomal protein L32

Chain 25:



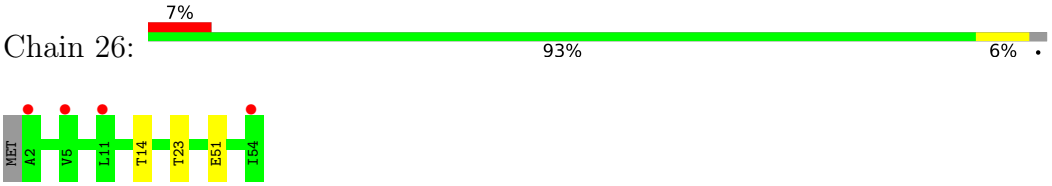
• Molecule 28: 50S ribosomal protein L33

Chain 16:



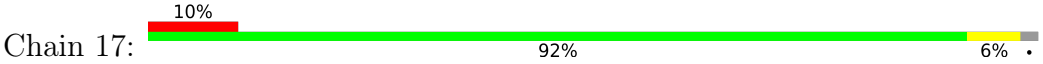
• Molecule 28: 50S ribosomal protein L33

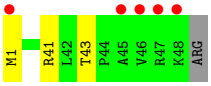
Chain 26:



• Molecule 29: 50S ribosomal protein L34

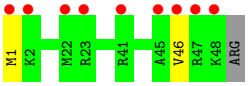
Chain 17:





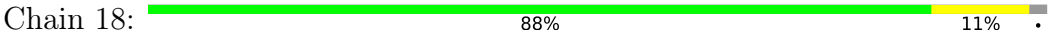
• Molecule 29: 50S ribosomal protein L34

Chain 27:



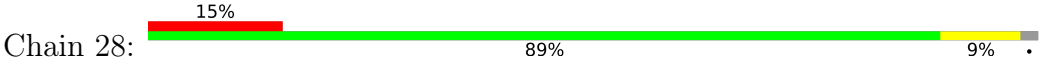
• Molecule 30: 50S ribosomal protein L35

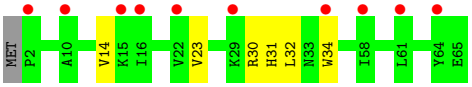
Chain 18:



• Molecule 30: 50S ribosomal protein L35

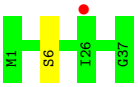
Chain 28:





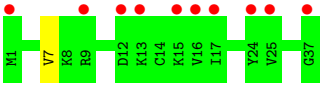
• Molecule 31: 50S ribosomal protein L36

Chain 19:



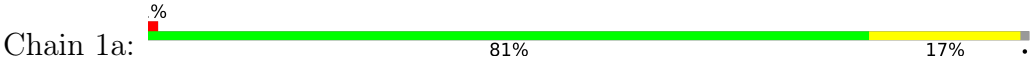
• Molecule 31: 50S ribosomal protein L36

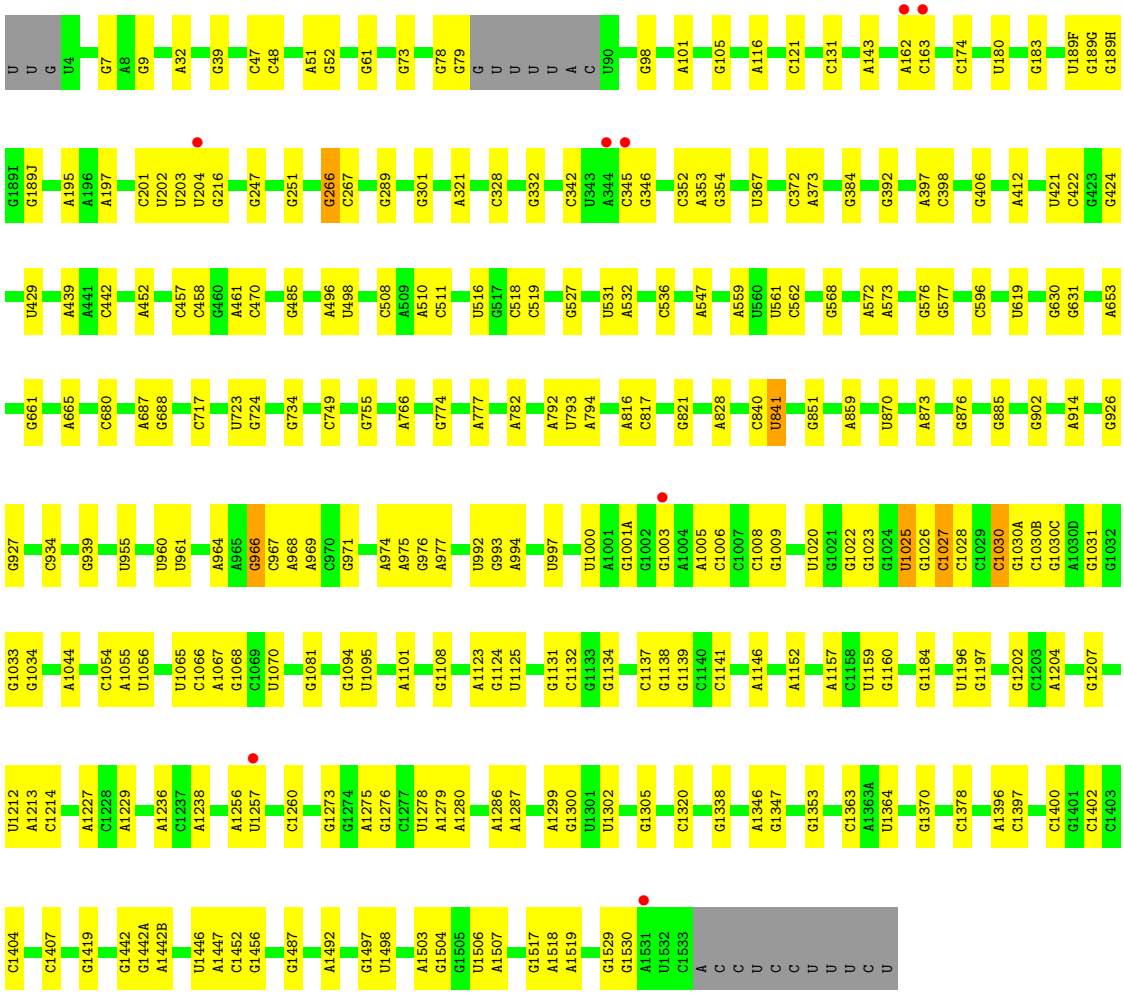
Chain 29:



• Molecule 32: 16S Ribosomal RNA

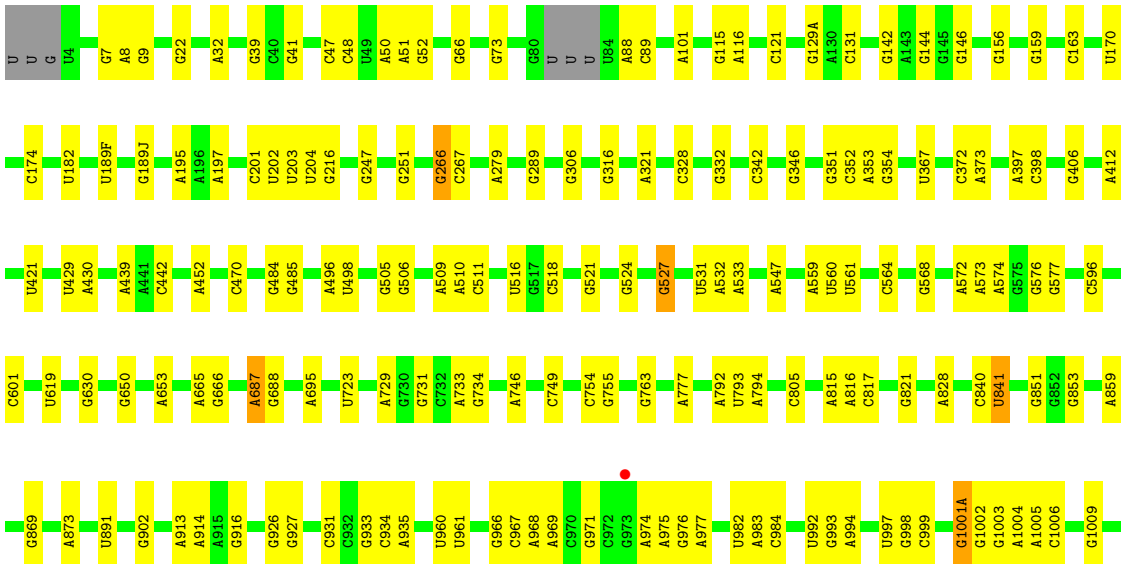
Chain 1a:

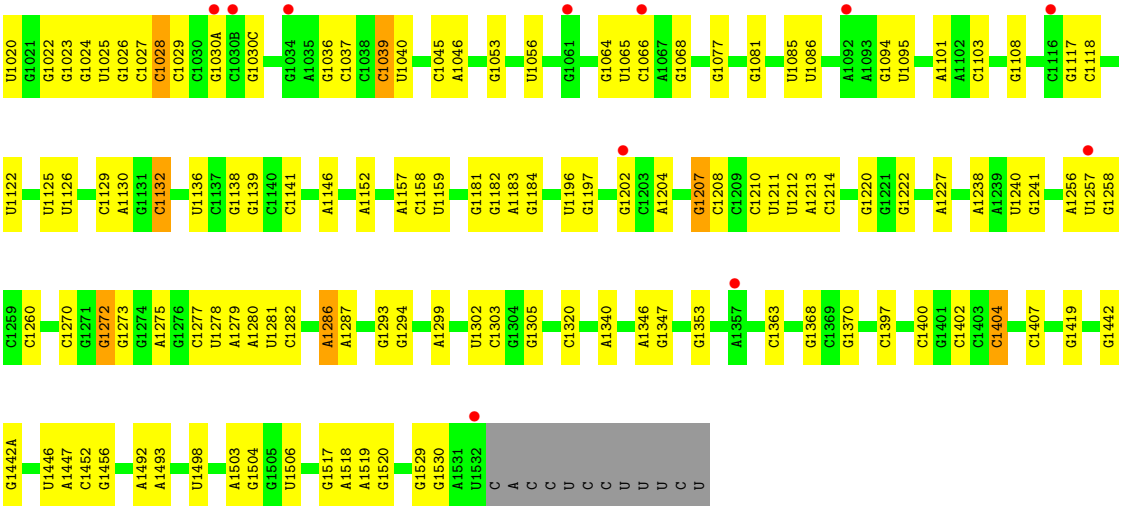




• Molecule 32: 16S Ribosomal RNA

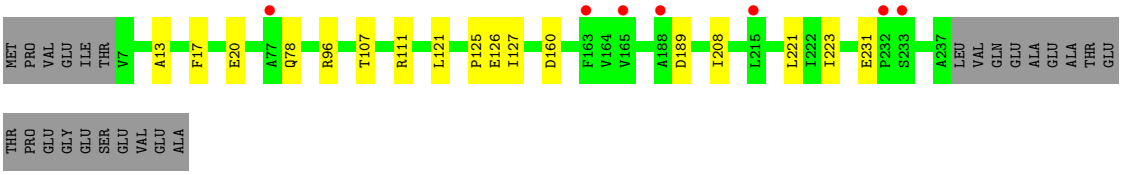
Chain 2a:





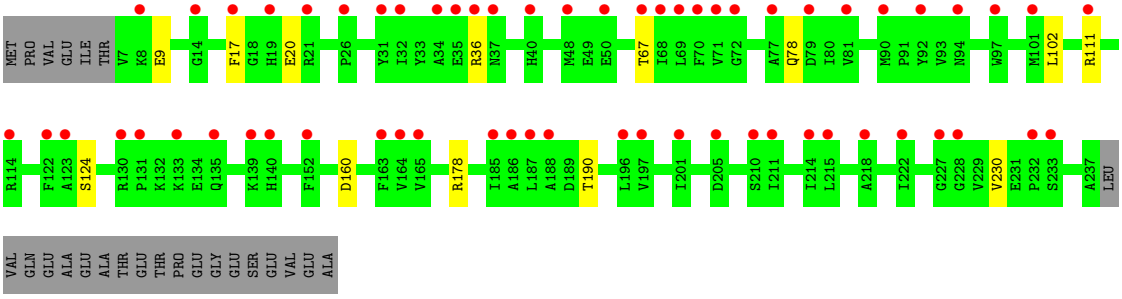
• Molecule 33: 30S ribosomal protein S2

Chain 1b:



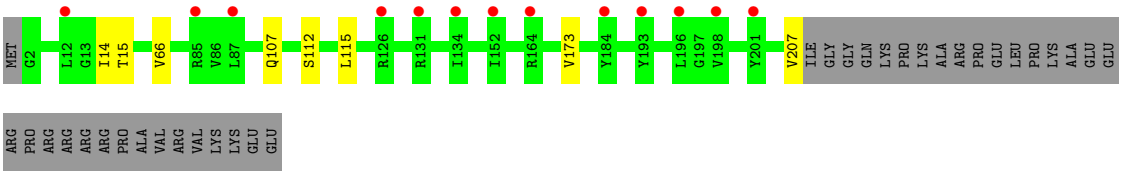
• Molecule 33: 30S ribosomal protein S2

Chain 2b:



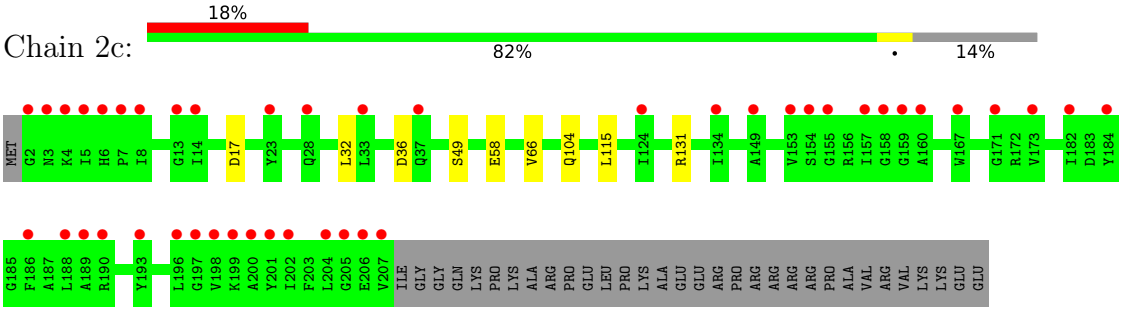
• Molecule 34: 30S ribosomal protein S3

Chain 1c:



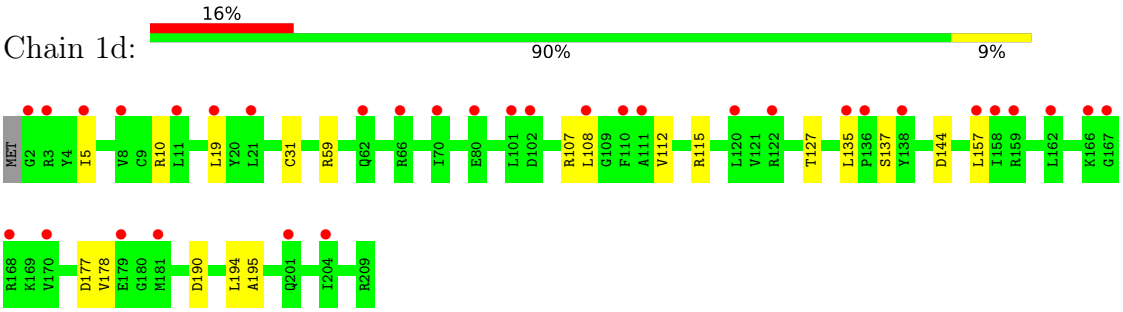
• Molecule 34: 30S ribosomal protein S3

Chain 2c:



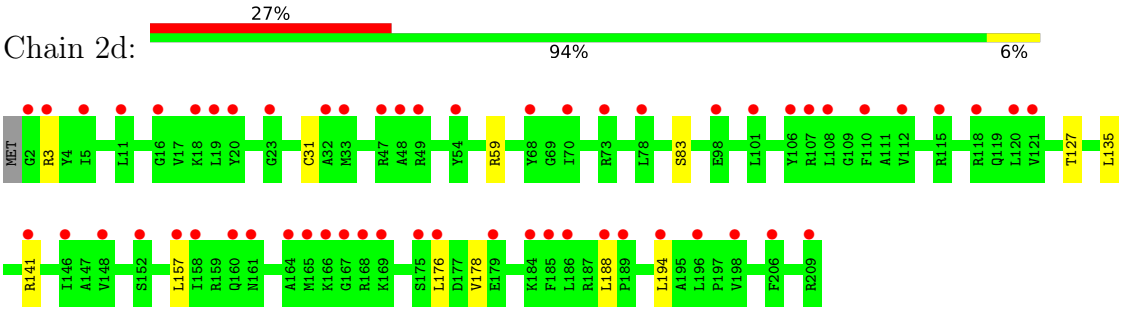
• Molecule 35: 30S ribosomal protein S4

Chain 1d:



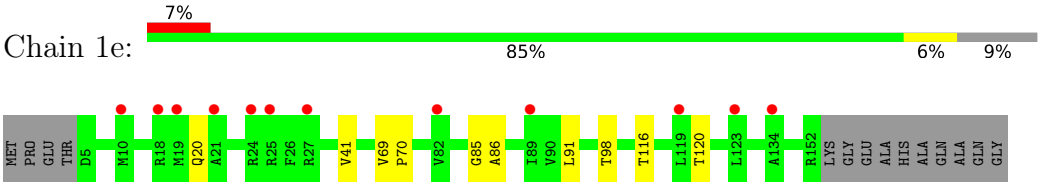
• Molecule 35: 30S ribosomal protein S4

Chain 2d:



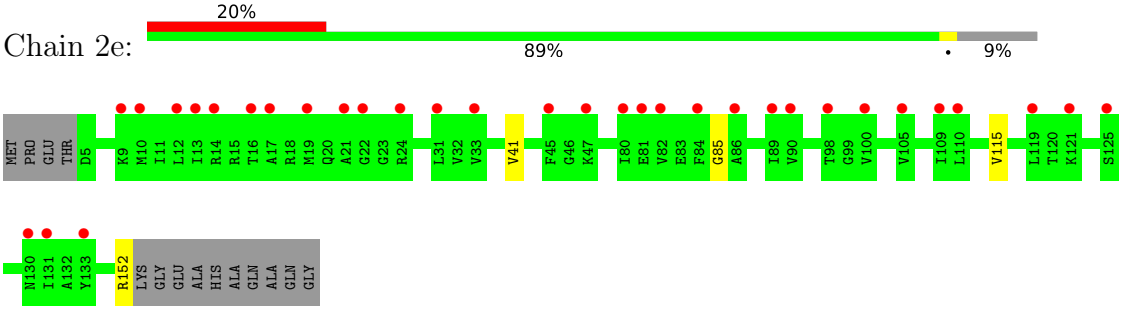
• Molecule 36: 30S ribosomal protein S5

Chain 1e:



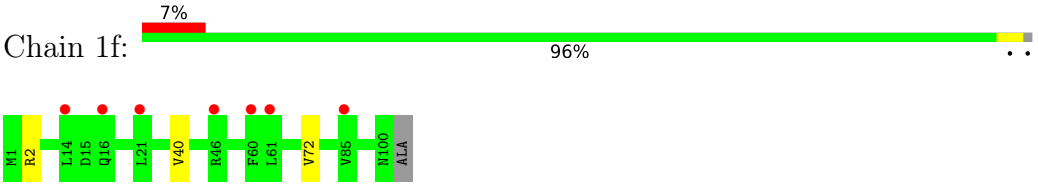
• Molecule 36: 30S ribosomal protein S5

Chain 2e:



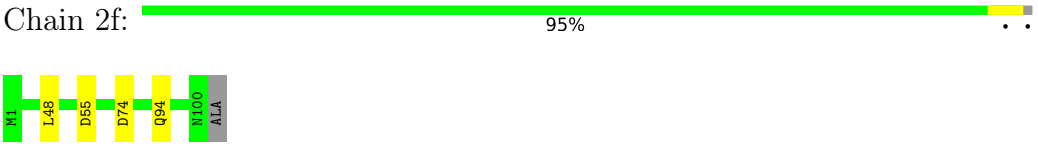
• Molecule 37: 30S ribosomal protein S6

Chain 1f:



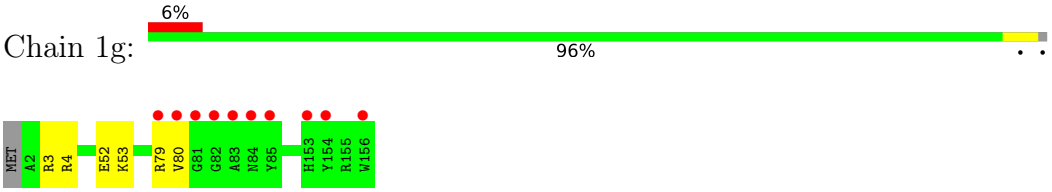
• Molecule 37: 30S ribosomal protein S6

Chain 2f:



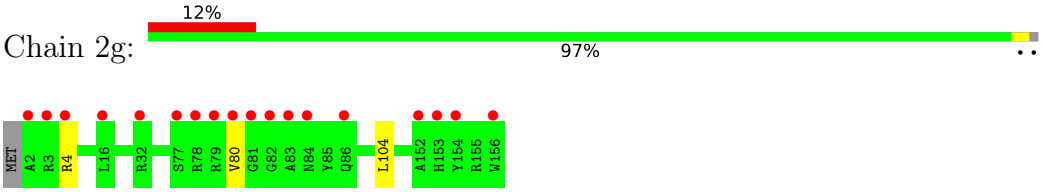
• Molecule 38: 30S ribosomal protein S7

Chain 1g:



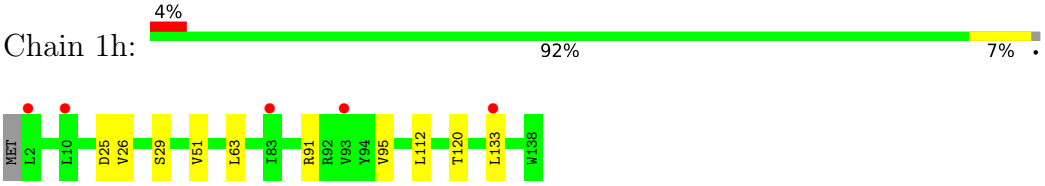
• Molecule 38: 30S ribosomal protein S7

Chain 2g:



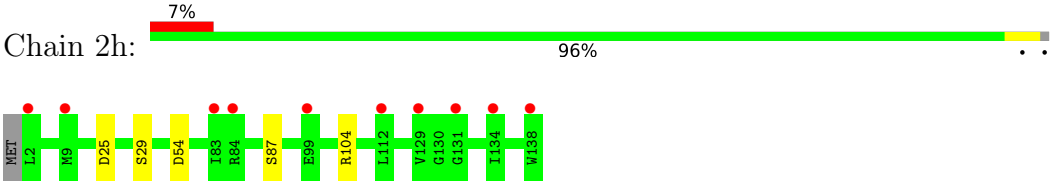
• Molecule 39: 30S ribosomal protein S8

Chain 1h:



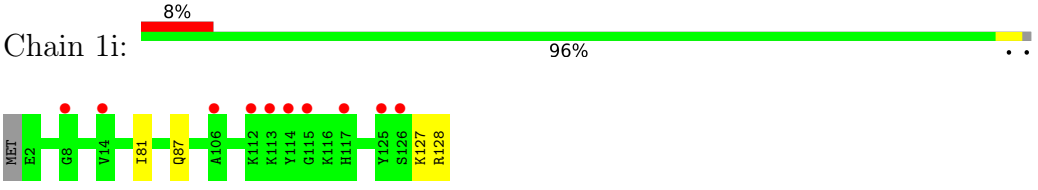
• Molecule 39: 30S ribosomal protein S8

Chain 2h:



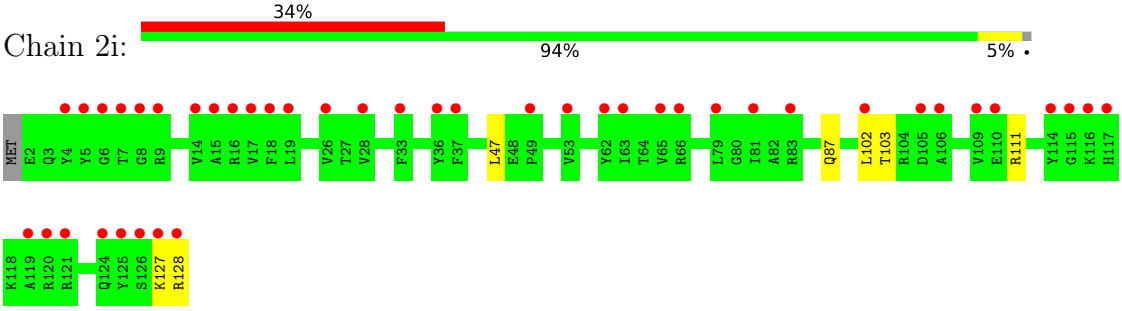
• Molecule 40: 30S ribosomal protein S9

Chain 1i:



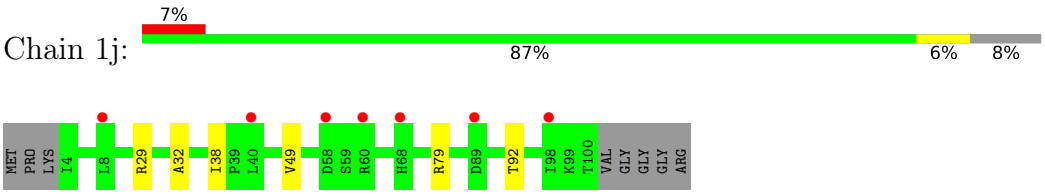
• Molecule 40: 30S ribosomal protein S9

Chain 2i:



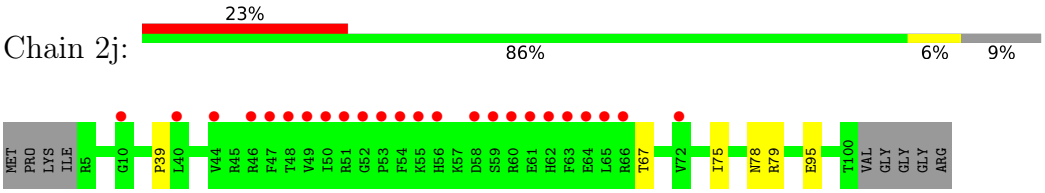
• Molecule 41: 30S ribosomal protein S10

Chain 1j:



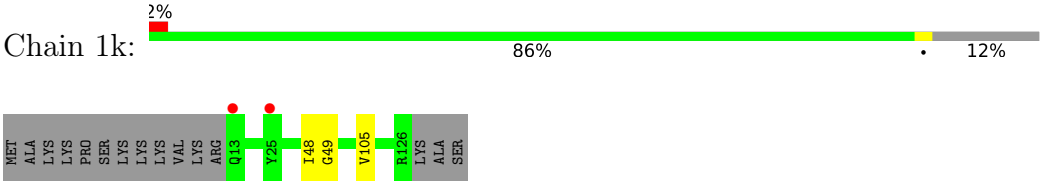
• Molecule 41: 30S ribosomal protein S10

Chain 2j:



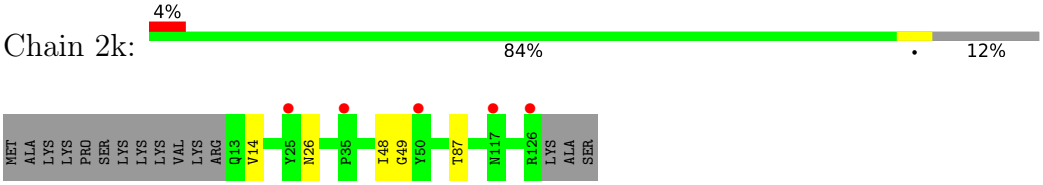
• Molecule 42: 30S ribosomal protein S11

Chain 1k:



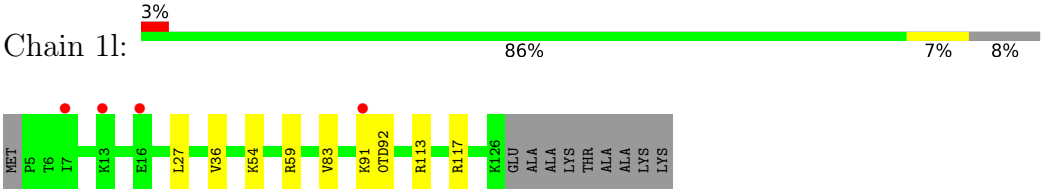
• Molecule 42: 30S ribosomal protein S11

Chain 2k:



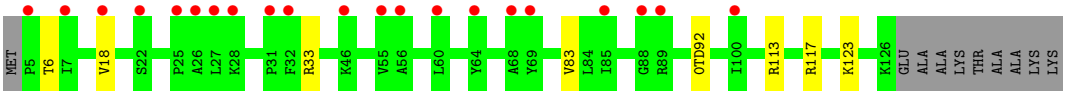
• Molecule 43: 30S ribosomal protein S12

Chain 1l:



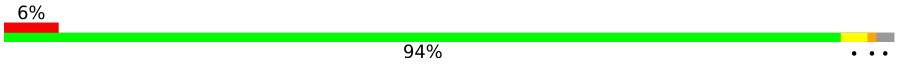
• Molecule 43: 30S ribosomal protein S12

Chain 2l:



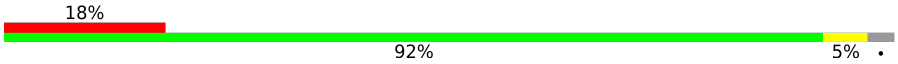
• Molecule 44: 30S ribosomal protein S13

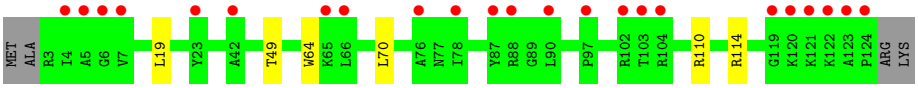
Chain 1m:



• Molecule 44: 30S ribosomal protein S13

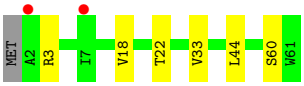
Chain 2m:





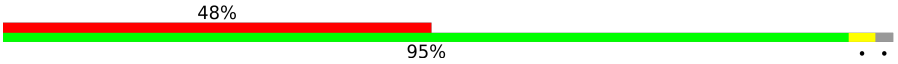
• Molecule 45: 30S ribosomal protein S14 type Z

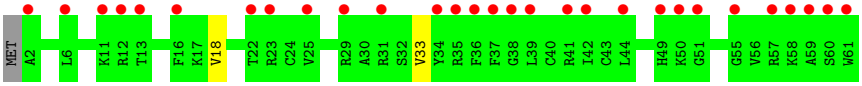
Chain 1n:



• Molecule 45: 30S ribosomal protein S14 type Z

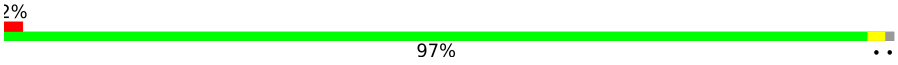
Chain 2n:





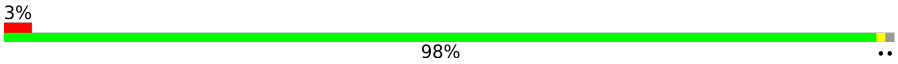
• Molecule 46: 30S ribosomal protein S15

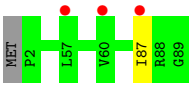
Chain 1o:



• Molecule 46: 30S ribosomal protein S15

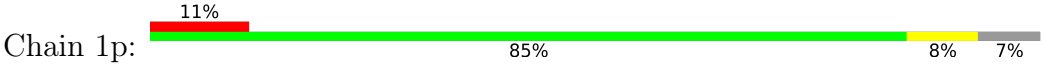
Chain 2o:

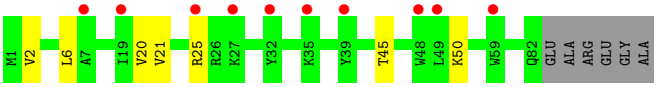




• Molecule 47: 30S ribosomal protein S16

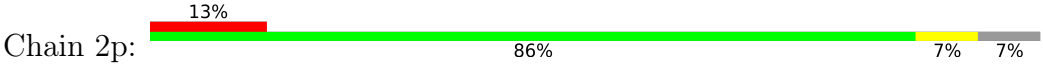
Chain 1p:





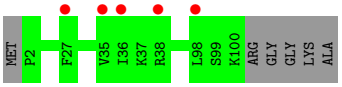
• Molecule 47: 30S ribosomal protein S16

Chain 2p:



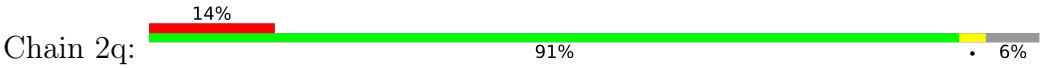
• Molecule 48: 30S ribosomal protein S17

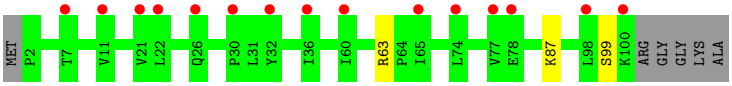
Chain 1q:



• Molecule 48: 30S ribosomal protein S17

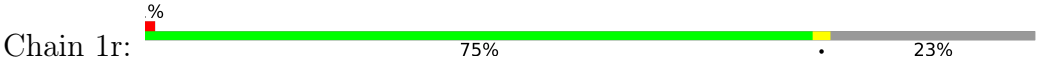
Chain 2q:





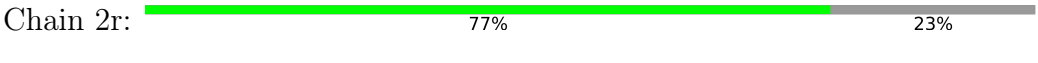
• Molecule 49: 30S ribosomal protein S18

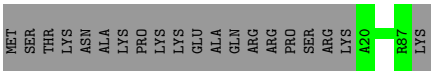
Chain 1r:



• Molecule 49: 30S ribosomal protein S18

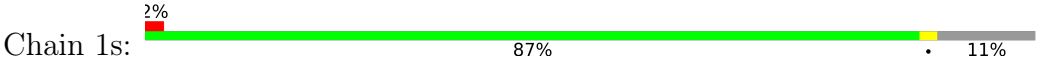
Chain 2r:

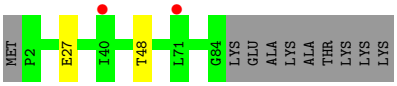




• Molecule 50: 30S ribosomal protein S19

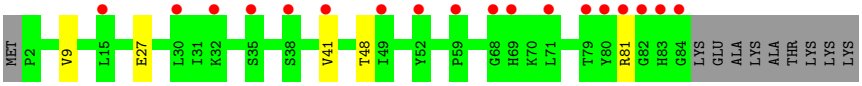
Chain 1s:





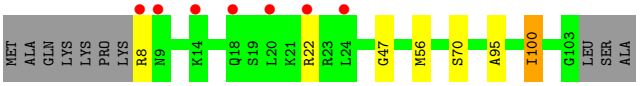
• Molecule 50: 30S ribosomal protein S19

Chain 2s:



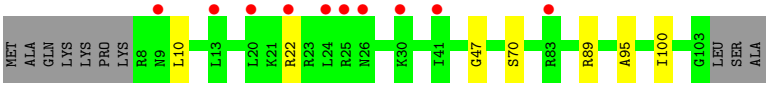
• Molecule 51: 30S ribosomal protein S20

Chain 1t:



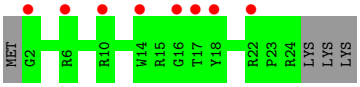
• Molecule 51: 30S ribosomal protein S20

Chain 2t:



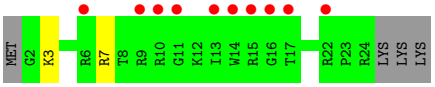
• Molecule 52: 30S ribosomal protein Thx

Chain 1u:



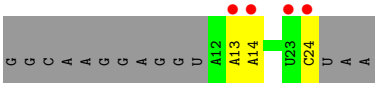
• Molecule 52: 30S ribosomal protein Thx

Chain 2u:



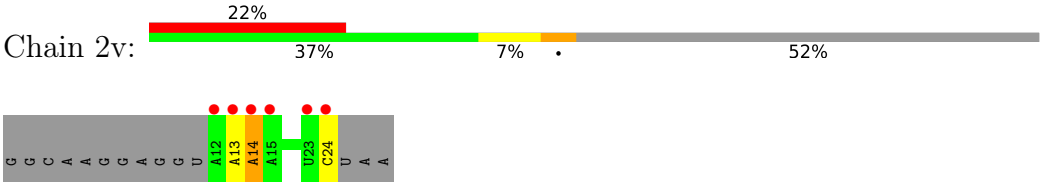
• Molecule 53: mRNA

Chain 1v:



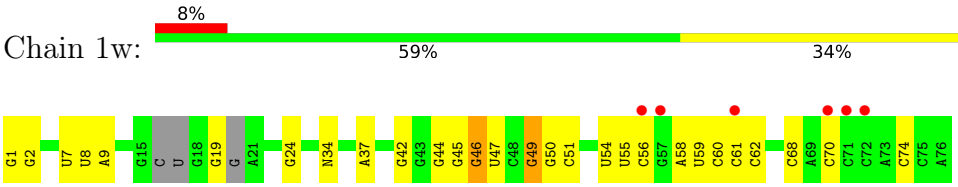
• Molecule 53: mRNA

Chain 2v:



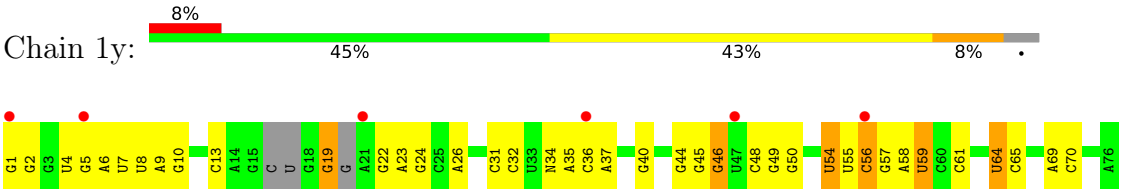
• Molecule 54: A-site and E-site tRNAs

Chain 1w:



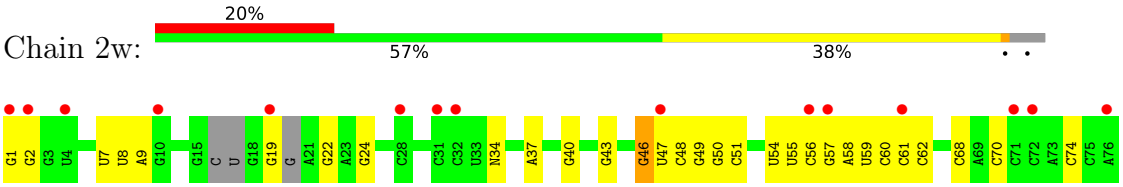
• Molecule 54: A-site and E-site tRNAs

Chain 1y:



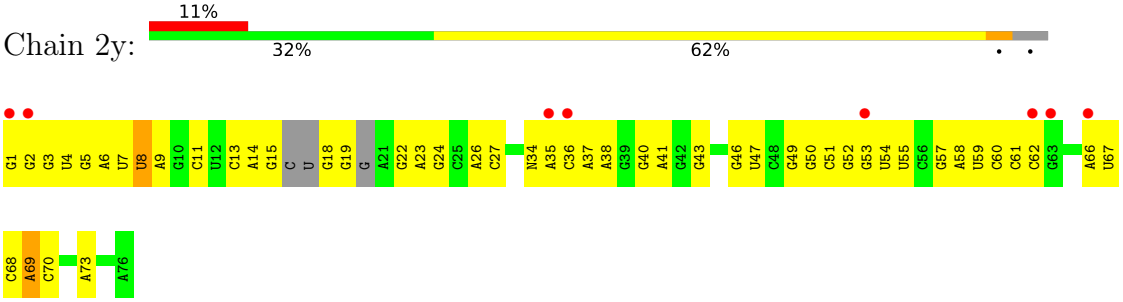
• Molecule 54: A-site and E-site tRNAs

Chain 2w:



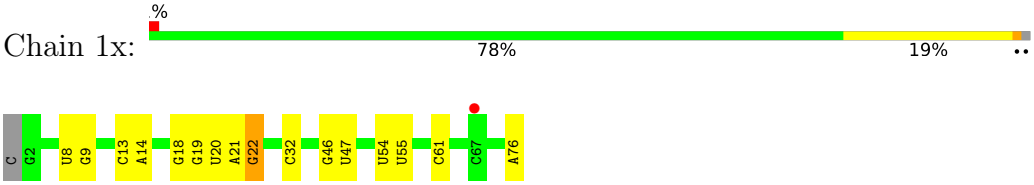
• Molecule 54: A-site and E-site tRNAs

Chain 2y:



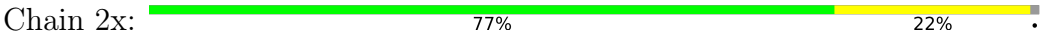
• Molecule 55: P-site tRNA

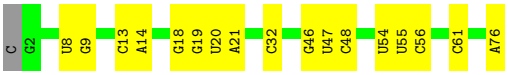
Chain 1x:



• Molecule 55: P-site tRNA

Chain 2x:




C
G2
U8
G9
C13
A14
G18
G19
U20
A21
C32
G46
U47
C48
U54
U55
C56
C61
A76

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	208.15Å 446.40Å 615.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	253.38 – 2.80 361.37 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (253.38-2.80) 99.8 (361.37-2.80)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.33 (at 2.82Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.215 , 0.263 0.215 , 0.263	Depositor DCC
R_{free} test set	69538 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	57.3	Xtriage
Anisotropy	0.245	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 52.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	300274	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.51% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, UR3, OMG, MA6, M2G, 5MC, K, 2MU, SF4, 0TD, PSU, 2MA, 7MG, 2MG, 6MZ, CM0, 5MU, 4OC, 4SU, DI0

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	0.54	0/69009	0.94	59/107712 (0.1%)
1	2A	0.41	0/67293	0.86	41/105034 (0.0%)
2	1B	0.45	1/2882 (0.0%)	0.85	0/4494
2	2B	0.38	1/2879 (0.0%)	0.82	1/4487 (0.0%)
3	1D	0.38	0/2186	0.55	0/2944
3	2D	0.33	0/2186	0.53	0/2944
4	1E	0.38	0/1592	0.56	0/2149
4	2E	0.31	0/1592	0.50	0/2149
5	1F	0.35	0/1619	0.54	0/2193
5	2F	0.31	0/1615	0.49	0/2188
6	1G	0.30	0/1448	0.51	0/1957
6	2G	0.29	0/1453	0.47	0/1963
7	1H	0.32	0/1356	0.50	0/1834
7	2H	0.28	0/1356	0.47	0/1834
8	1I	0.29	0/1112	0.46	0/1514
8	2I	0.29	0/1079	0.49	0/1475
9	1N	0.34	0/1144	0.50	0/1543
9	2N	0.28	0/1144	0.47	0/1543
10	1O	0.38	0/943	0.54	0/1269
10	2O	0.33	0/943	0.52	0/1269
11	1P	0.34	0/1152	0.54	0/1533
11	2P	0.30	0/1152	0.51	0/1533
12	1Q	0.36	0/1143	0.51	0/1527
12	2Q	0.30	0/1143	0.48	0/1527
13	1R	0.34	0/982	0.54	0/1312
13	2R	0.27	0/982	0.50	0/1312
14	1S	0.31	0/883	0.53	0/1176
14	2S	0.30	0/880	0.47	0/1172
15	1T	0.33	0/1105	0.52	0/1477
15	2T	0.31	0/1097	0.47	0/1468
16	1U	0.40	0/977	0.50	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	2U	0.30	0/977	0.44	0/1301
17	1V	0.37	0/782	0.56	0/1049
17	2V	0.30	0/782	0.50	0/1049
18	1W	0.35	0/897	0.52	0/1205
18	2W	0.32	0/897	0.49	0/1205
19	1X	0.37	0/764	0.55	0/1025
19	2X	0.31	0/764	0.47	0/1025
20	1Y	0.33	0/819	0.51	0/1095
20	2Y	0.32	0/819	0.52	0/1095
21	1Z	0.34	0/1267	0.52	0/1717
21	2Z	0.29	0/1299	0.50	0/1763
22	10	0.36	0/662	0.57	0/881
22	20	0.31	0/662	0.52	0/881
23	11	0.35	0/762	0.52	0/1014
23	21	0.32	0/762	0.50	0/1014
24	12	0.32	0/590	0.48	0/781
24	22	0.28	0/590	0.39	0/781
25	13	0.33	0/474	0.52	0/635
25	23	0.32	0/469	0.45	0/630
26	14	0.35	0/565	0.70	1/761 (0.1%)
26	24	0.33	0/545	0.56	0/737
27	15	0.36	0/469	0.56	0/635
27	25	0.35	0/469	0.50	0/635
28	16	0.37	0/460	0.55	0/613
28	26	0.32	0/456	0.51	0/608
29	17	0.36	0/426	0.50	0/561
29	27	0.32	0/426	0.52	0/561
30	18	0.34	0/525	0.56	0/691
30	28	0.29	0/525	0.48	0/691
31	19	0.35	0/310	0.56	0/407
31	29	0.28	0/310	0.54	0/407
32	1a	0.39	0/35795	0.87	26/55864 (0.0%)
32	2a	0.35	0/35886	0.87	40/56005 (0.1%)
33	1b	0.29	0/1881	0.47	0/2542
33	2b	0.30	0/1860	0.48	0/2518
34	1c	0.35	1/1572 (0.1%)	0.45	0/2126
34	2c	0.29	0/1566	0.47	0/2119
35	1d	0.30	0/1685	0.50	1/2262 (0.0%)
35	2d	0.30	0/1704	0.46	0/2284
36	1e	0.31	0/1145	0.49	0/1543
36	2e	0.30	0/1149	0.50	0/1548
37	1f	0.29	0/823	0.46	0/1115
37	2f	0.32	0/829	0.46	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	1g	0.28	0/1250	0.43	0/1679
38	2g	0.28	0/1254	0.43	0/1683
39	1h	0.29	0/1108	0.49	0/1494
39	2h	0.28	0/1108	0.46	0/1494
40	1i	0.30	0/1002	0.49	0/1346
40	2i	0.29	0/997	0.49	0/1343
41	1j	0.27	0/722	0.48	0/982
41	2j	0.28	0/727	0.48	0/988
42	1k	0.29	0/844	0.49	0/1145
42	2k	0.29	0/848	0.47	0/1149
43	1l	0.30	0/937	0.51	0/1260
43	2l	0.28	0/937	0.49	0/1260
44	1m	0.29	0/969	0.49	0/1302
44	2m	0.27	0/961	0.47	0/1291
45	1n	0.31	0/501	0.52	0/664
45	2n	0.29	0/501	0.45	0/664
46	1o	0.29	0/739	0.46	0/985
46	2o	0.25	0/739	0.45	0/985
47	1p	0.29	0/697	0.52	0/939
47	2p	0.30	0/693	0.49	0/935
48	1q	0.29	0/836	0.47	0/1117
48	2q	0.28	0/836	0.46	0/1117
49	1r	0.28	0/560	0.48	0/746
49	2r	0.26	0/560	0.47	0/746
50	1s	0.27	0/667	0.53	0/900
50	2s	0.30	0/661	0.52	0/893
51	1t	0.28	0/730	0.41	0/965
51	2t	0.27	0/729	0.44	0/965
52	1u	0.29	0/203	0.49	0/266
52	2u	0.40	0/203	0.54	0/266
53	1v	0.49	0/308	1.04	0/477
53	2v	0.51	0/308	1.06	2/477 (0.4%)
54	1w	0.74	5/1600 (0.3%)	1.28	14/2482 (0.6%)
54	1y	0.76	4/1600 (0.2%)	1.36	21/2482 (0.8%)
54	2w	0.52	1/1600 (0.1%)	1.05	2/2482 (0.1%)
54	2y	0.66	2/1600 (0.1%)	1.31	20/2482 (0.8%)
55	1x	0.50	1/1725 (0.1%)	1.03	8/2689 (0.3%)
55	2x	0.42	0/1725	0.99	3/2689 (0.1%)
All	All	0.42	16/316731 (0.0%)	0.82	239/474164 (0.1%)

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

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
26	14	0	3
26	24	0	1
33	2b	0	1
All	All	0	5

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1y	59	U	C4-O4	13.34	1.34	1.23
54	1w	59	U	C4-O4	13.21	1.34	1.23
54	1y	32	C	C4-N4	-10.96	1.24	1.33
54	1w	60	C	C4-N4	-10.56	1.24	1.33
2	2B	1	U	OP3-P	-10.41	1.48	1.61
54	2w	1	G	OP3-P	-10.32	1.48	1.61
54	1w	1	G	OP3-P	-10.29	1.48	1.61
54	1y	1	G	OP3-P	-10.25	1.48	1.61
54	2y	1	G	OP3-P	-10.20	1.49	1.61
2	1B	1	U	OP3-P	-10.04	1.49	1.61
34	1c	173	VAL	C-N	7.84	1.49	1.34
54	1y	32	C	N3-C4	7.09	1.39	1.33
54	1w	60	C	N3-C4	6.75	1.38	1.33
55	1x	14	A	C8-N7	-5.33	1.27	1.31
54	1w	59	U	N3-C4	-5.29	1.33	1.38
54	2y	69	A	N9-C4	5.10	1.41	1.37

All (239) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	1w	60	C	N3-C4-C5	-21.13	113.45	121.90
54	1y	32	C	N3-C4-C5	-19.48	114.11	121.90
54	1w	60	C	C2-N3-C4	16.40	128.10	119.90
54	1y	32	C	C2-N3-C4	14.90	127.35	119.90
54	1y	59	U	C2-N3-C4	-11.70	119.98	127.00
54	1y	59	U	N3-C4-C5	11.48	121.49	114.60
54	1w	59	U	N3-C4-C5	11.16	121.30	114.60
54	1w	59	U	C2-N3-C4	-10.57	120.66	127.00
1	1A	1086	A	N1-C6-N6	-9.94	112.63	118.60
54	1w	60	C	C5-C4-N4	9.76	127.03	120.20
1	1A	1639	U	O5'-P-OP2	-9.55	97.11	105.70
54	1w	60	C	N1-C2-O2	9.24	124.44	118.90
54	1y	59	U	C5-C4-O4	-8.97	120.52	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	1158	C	C2-N1-C1'	8.75	128.43	118.80
32	2a	841	U	C2-N1-C1'	8.58	127.99	117.70
54	1y	50	G	C5-C6-O6	8.36	133.61	128.60
32	2a	1001(A)	G	N3-C4-N9	8.33	131.00	126.00
1	1A	1075	C	N1-C2-O2	8.31	123.89	118.90
54	1y	64	U	N1-C2-O2	-8.30	116.99	122.80
54	1w	59	U	C5-C4-O4	-8.28	120.93	125.90
54	1y	32	C	C5-C4-N4	8.28	126.00	120.20
53	2v	14	A	N1-C6-N6	8.24	123.54	118.60
54	1y	32	C	N1-C2-O2	8.12	123.77	118.90
32	2a	1158	C	N1-C2-O2	8.08	123.75	118.90
1	1A	1614	A	O5'-P-OP1	-8.02	98.49	105.70
1	2A	2473	U	C2-N1-C1'	7.96	127.26	117.70
54	1y	59	U	N1-C2-N3	7.95	119.67	114.90
55	1x	14	A	C5-N7-C8	7.86	107.83	103.90
55	2x	14	A	C5-N7-C8	7.86	107.83	103.90
54	2y	69	A	C6-N1-C2	-7.85	113.89	118.60
54	2y	23	A	N1-C6-N6	7.82	123.30	118.60
2	2B	80	U	O4'-C1'-N1	7.81	114.45	108.20
32	1a	1025	U	N1-C2-O2	7.63	128.14	122.80
54	1w	59	U	N1-C2-N3	7.59	119.45	114.90
55	1x	14	A	C4-C5-C6	7.54	120.77	117.00
26	14	64	GLY	N-CA-C	7.51	131.89	113.10
54	2y	4	U	C5-C4-O4	-7.50	121.40	125.90
32	1a	1027	C	C6-N1-C1'	7.48	129.78	120.80
1	1A	512	G	O4'-C1'-N9	7.47	114.18	108.20
54	2y	68	C	N1-C2-O2	7.47	123.38	118.90
32	1a	1027	C	N3-C4-C5	-7.41	118.94	121.90
1	2A	1828	G	O5'-P-OP1	-7.38	99.05	105.70
1	1A	1776	G	O5'-P-OP2	-7.31	99.12	105.70
1	1A	1075	C	C2-N3-C4	7.28	123.54	119.90
1	1A	2789	C	O4'-C1'-N1	7.28	114.02	108.20
54	2y	50	G	C5-C6-O6	7.24	132.94	128.60
32	2a	841	U	C5-C6-N1	7.19	126.29	122.70
1	1A	2167	U	N3-C2-O2	-7.14	117.20	122.20
32	2a	754	C	C2-N1-C1'	7.08	126.59	118.80
32	1a	1027	C	C2-N1-C1'	-7.04	111.05	118.80
1	2A	2167	U	N3-C2-O2	-7.03	117.28	122.20
1	2A	2167	U	N1-C2-O2	7.03	127.72	122.80
32	1a	1025	U	C2-N1-C1'	7.00	126.10	117.70
1	1A	2589	A	O5'-P-OP2	6.95	119.03	110.70
32	1a	841	U	C2-N1-C1'	6.93	126.02	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	754	C	N1-C2-O2	6.93	123.06	118.90
1	2A	2136	C	N1-C2-O2	6.91	123.05	118.90
32	1a	841	U	C5-C6-N1	6.87	126.14	122.70
1	1A	12	U	C2-N1-C1'	6.81	125.88	117.70
1	1A	2167	U	N1-C2-O2	6.78	127.55	122.80
54	1y	56	C	N1-C2-O2	6.75	122.95	118.90
32	2a	1001(A)	G	C4-N9-C1'	6.72	135.24	126.50
32	1a	1030(B)	C	C2-N1-C1'	6.71	126.18	118.80
32	2a	1039	C	C2-N1-C1'	6.70	126.17	118.80
1	1A	226	G	O4'-C1'-N9	6.68	113.54	108.20
32	2a	1126	U	C2-N1-C1'	6.66	125.69	117.70
53	2v	14	A	C5-C6-N6	-6.66	118.37	123.70
55	1x	46	G	C6-N1-C2	-6.64	121.12	125.10
1	1A	2167	U	C2-N1-C1'	6.61	125.63	117.70
1	1A	975	C	N1-C2-O2	-6.51	114.99	118.90
32	1a	1030	C	N1-C2-O2	6.47	122.78	118.90
1	2A	2155	G	N3-C4-N9	6.46	129.88	126.00
1	1A	1174	A	OP1-P-O3'	6.43	119.36	105.20
1	1A	1176	G	OP1-P-O3'	6.39	119.25	105.20
54	1w	49	G	N3-C4-N9	6.38	129.83	126.00
32	2a	1001(A)	G	C8-N9-C1'	-6.37	118.72	127.00
54	1y	56	C	C2-N3-C4	6.31	123.06	119.90
32	1a	1030(B)	C	N1-C2-O2	6.29	122.67	118.90
1	2A	1992	G	P-O3'-C3'	6.27	127.22	119.70
54	1y	64	U	C2-N1-C1'	-6.26	110.18	117.70
1	1A	2682	U	O5'-P-OP2	-6.25	100.08	105.70
1	2A	2167	U	C2-N1-C1'	6.22	125.17	117.70
1	1A	800	A	O5'-P-OP1	-6.13	100.18	105.70
54	2y	69	A	N3-C4-N9	6.10	132.28	127.40
32	2a	1158	C	C6-N1-C1'	-6.06	113.53	120.80
1	1A	845	G	O4'-C1'-N9	6.06	113.05	108.20
54	1y	50	G	C6-N1-C2	6.05	128.73	125.10
1	2A	2473	U	N1-C2-O2	6.05	127.03	122.80
54	2y	23	A	C5-C6-N6	-6.03	118.88	123.70
32	1a	1027	C	C5-C4-N4	6.03	124.42	120.20
1	1A	1063	G	C5-C6-O6	6.01	132.21	128.60
1	1A	1992	G	P-O3'-C3'	6.00	126.91	119.70
32	2a	1001(A)	G	C6-C5-N7	-6.00	126.80	130.40
32	2a	1039	C	C5-C4-N4	-5.98	116.01	120.20
55	1x	14	A	C5-C6-N1	-5.97	114.72	117.70
1	1A	1177	A	O5'-P-OP1	-5.95	100.34	105.70
1	1A	2789	C	C2-N1-C1'	-5.93	112.28	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	2x	14	A	C4-C5-C6	5.93	119.97	117.00
1	1A	2848	G	O4'-C1'-N9	5.93	112.94	108.20
1	1A	2712(A)	A	O5'-P-OP1	-5.91	100.39	105.70
32	2a	1158	C	N3-C2-O2	-5.89	117.78	121.90
1	2A	1204	A	O4'-C1'-N9	5.88	112.90	108.20
32	1a	1034	G	C6-N1-C2	5.88	128.63	125.10
1	2A	787	U	O5'-P-OP1	-5.86	100.42	105.70
1	2A	2174	C	C2-N1-C1'	5.85	125.23	118.80
55	1x	14	A	C8-N9-C1'	-5.81	117.24	127.70
54	2y	4	U	C2-N3-C4	-5.80	123.52	127.00
1	1A	1063	G	C6-N1-C2	5.80	128.58	125.10
32	2a	841	U	C6-N1-C2	-5.80	117.52	121.00
54	1w	60	C	C5-C6-N1	5.79	123.89	121.00
54	1y	32	C	N1-C2-N3	-5.78	115.15	119.20
32	2a	1001(A)	G	N3-C4-C5	-5.77	125.71	128.60
32	1a	266	G	P-O3'-C3'	5.75	126.59	119.70
1	1A	1313	U	C2-N1-C1'	5.74	124.59	117.70
32	1a	841	U	C6-N1-C2	-5.72	117.57	121.00
55	1x	14	A	C4-N9-C1'	5.72	136.60	126.30
32	2a	266	G	P-O3'-C3'	5.71	126.55	119.70
32	2a	1025	U	N1-C2-O2	5.69	126.78	122.80
32	2a	1158	C	C6-N1-C2	-5.67	118.03	120.30
32	2a	1158	C	C5-C6-N1	5.62	123.81	121.00
32	2a	869	G	N1-C6-O6	5.61	123.27	119.90
1	1A	881	G	C4-N9-C1'	5.61	133.79	126.50
1	2A	1380	G	O5'-P-OP2	-5.61	100.65	105.70
54	2y	69	A	C5-C6-N6	-5.61	119.22	123.70
32	1a	1067	A	P-O3'-C3'	5.59	126.41	119.70
54	1w	60	C	N1-C2-N3	-5.58	115.30	119.20
54	1y	19	G	C6-N1-C2	5.58	128.44	125.10
54	2y	50	G	N1-C6-O6	-5.56	116.56	119.90
1	1A	1174	A	P-O3'-C3'	5.54	126.35	119.70
1	1A	1082	U	N3-C4-O4	-5.54	115.53	119.40
32	1a	1034	G	C5-C6-O6	5.52	131.91	128.60
1	1A	784	A	O4'-C1'-N9	5.51	112.61	108.20
32	2a	1025	U	C2-N1-C1'	5.51	124.31	117.70
1	1A	881	G	C6-C5-N7	-5.50	127.10	130.40
1	1A	1063	G	N3-C2-N2	5.49	123.74	119.90
1	2A	214	G	O4'-C1'-N9	5.48	112.58	108.20
54	1w	44	G	P-O3'-C3'	5.47	126.26	119.70
1	2A	2501	C	C2-N1-C1'	-5.46	112.79	118.80
1	2A	2140	C	N1-C2-O2	5.45	122.17	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	1y	64	U	C6-N1-C1'	5.45	128.82	121.20
54	2y	69	A	C5-C6-N1	5.44	120.42	117.70
32	1a	266	G	O4'-C1'-N9	-5.43	103.86	108.20
32	2a	1039	C	N1-C2-O2	5.42	122.15	118.90
1	2A	383	U	O4'-C1'-N1	5.41	112.52	108.20
1	1A	975	C	C2-N1-C1'	-5.40	112.86	118.80
32	2a	754	C	C6-N1-C1'	-5.40	114.32	120.80
1	2A	1420	U	P-O3'-C3'	5.38	126.16	119.70
1	1A	1058	G	C5-C6-O6	5.38	131.82	128.60
54	2y	60	C	C2-N1-C1'	5.37	124.71	118.80
1	1A	1379	A	C8-N9-C4	5.37	107.95	105.80
32	2a	1039	C	C6-N1-C1'	-5.37	114.36	120.80
1	1A	570	G	C5-C6-O6	-5.37	125.38	128.60
54	2y	67	U	C5-C6-N1	5.37	125.38	122.70
32	2a	1272	G	C4-N9-C1'	5.36	133.47	126.50
32	1a	1030(B)	C	C6-N1-C2	-5.36	118.16	120.30
1	2A	2136	C	C2-N1-C1'	5.35	124.68	118.80
1	1A	1086	A	C5-C6-N1	5.35	120.37	117.70
1	2A	2689	U	P-O3'-C3'	5.35	126.11	119.70
1	2A	1313	U	C2-N1-C1'	5.33	124.09	117.70
35	1d	195	ALA	C-N-CA	-5.33	108.38	121.70
32	1a	1025	U	C6-N1-C1'	-5.32	113.75	121.20
1	2A	1644	C	C2-N1-C1'	5.32	124.65	118.80
1	1A	2589	A	O5'-P-OP1	-5.31	100.92	105.70
1	1A	2593	U	N3-C4-O4	-5.30	115.69	119.40
1	1A	2873	A	O4'-C1'-N9	5.29	112.44	108.20
55	1x	22	G	C5-N7-C8	-5.29	101.65	104.30
54	1y	4	U	C5-C4-O4	-5.29	122.72	125.90
32	2a	1001(A)	G	N9-C4-C5	-5.29	103.28	105.40
1	2A	512	G	O4'-C1'-N9	5.29	112.43	108.20
1	2A	1698	A	O4'-C1'-N9	5.29	112.43	108.20
32	2a	841	U	N1-C2-O2	5.29	126.50	122.80
1	1A	2319	G	O4'-C1'-N9	5.28	112.43	108.20
1	2A	528	A	P-O3'-C3'	5.28	126.04	119.70
32	2a	687	A	P-O3'-C3'	5.28	126.03	119.70
1	1A	576	U	O5'-P-OP1	-5.27	100.95	105.70
1	2A	2473	U	C6-N1-C1'	-5.27	113.82	121.20
54	2y	18	G	C4-N9-C1'	5.27	133.36	126.50
54	2w	61	C	C2-N1-C1'	5.27	124.60	118.80
32	2a	1029	C	N1-C2-O2	5.27	122.06	118.90
1	2A	141	A	N7-C8-N9	5.26	116.43	113.80
1	1A	2789	C	C6-N1-C1'	5.25	127.10	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	2y	69	A	N3-C4-C5	-5.25	123.13	126.80
1	2A	2473	U	N3-C2-O2	-5.24	118.53	122.20
1	2A	928	G	C5-C6-O6	-5.22	125.47	128.60
1	2A	928	G	N1-C6-O6	5.22	123.03	119.90
54	1y	19	G	C5-C6-O6	5.21	131.73	128.60
32	1a	955	U	C2-N3-C4	5.21	130.13	127.00
32	1a	782	A	O5'-P-OP1	-5.21	101.02	105.70
54	2y	60	C	N1-C2-O2	5.20	122.02	118.90
54	2y	27	C	N1-C2-O2	5.20	122.02	118.90
1	2A	928	G	C6-C5-N7	-5.19	127.28	130.40
1	2A	2206	G	C4-N9-C1'	-5.19	119.75	126.50
54	1w	49	G	N3-C4-C5	-5.19	126.00	128.60
1	2A	2155	G	C6-C5-N7	-5.18	127.29	130.40
32	2a	115	G	P-O3'-C3'	5.17	125.90	119.70
32	1a	841	U	N1-C2-O2	5.16	126.41	122.80
1	1A	881	G	N7-C8-N9	5.16	115.68	113.10
1	2A	1558	A	C2-N3-C4	-5.16	108.02	110.60
32	1a	841	U	N3-C2-O2	-5.16	118.59	122.20
1	1A	2032	G	C5-N7-C8	5.16	106.88	104.30
1	1A	2036	C	O5'-P-OP1	-5.14	101.07	105.70
1	1A	2615	U	O5'-P-OP1	-5.14	101.07	105.70
1	2A	2689	U	N3-C2-O2	-5.14	118.60	122.20
54	2y	67	U	C2-N1-C1'	5.14	123.87	117.70
54	1y	22	G	N1-C6-O6	5.13	122.98	119.90
1	2A	228	A	P-O3'-C3'	5.13	125.86	119.70
32	2a	1132	C	N3-C2-O2	-5.13	118.31	121.90
1	1A	2207	G	C4-N9-C1'	5.13	133.16	126.50
32	2a	754	C	N3-C2-O2	-5.12	118.31	121.90
32	2a	266	G	N3-C4-C5	-5.12	126.04	128.60
32	1a	1123	A	C5-C6-N6	5.12	127.80	123.70
54	2w	61	C	C6-N1-C2	-5.11	118.26	120.30
32	2a	1126	U	N1-C2-O2	5.11	126.38	122.80
32	2a	1028	C	C2-N3-C4	5.11	122.45	119.90
1	1A	1075	C	C5-C4-N4	5.11	123.77	120.20
1	2A	528	A	OP1-P-O3'	5.10	116.42	105.20
1	1A	2723	C	C6-N1-C2	-5.10	118.26	120.30
1	2A	2447	G	C4-N9-C1'	-5.09	119.88	126.50
32	2a	1286	A	N7-C8-N9	5.09	116.34	113.80
54	2y	68	C	N3-C2-O2	-5.09	118.34	121.90
1	1A	1080	C	C2-N3-C4	5.08	122.44	119.90
32	2a	913	A	P-O3'-C3'	5.08	125.79	119.70
1	1A	1210	A	P-O3'-C3'	5.07	125.78	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	171	G	C4-N9-C1'	5.07	133.09	126.50
1	2A	2473	U	C5-C6-N1	5.07	125.23	122.70
32	1a	1030(B)	C	N3-C2-O2	-5.07	118.35	121.90
32	2a	841	U	N3-C2-O2	-5.06	118.66	122.20
1	1A	2501	C	C2-N1-C1'	-5.05	113.24	118.80
55	2x	46	G	N3-C2-N2	-5.05	116.37	119.90
1	1A	1969	A	OP1-P-O3'	5.04	116.28	105.20
1	1A	2371	G	C5-C6-N1	5.04	114.02	111.50
32	1a	266	G	C4-N9-C1'	5.02	133.03	126.50
54	1w	60	C	C4-C5-C6	5.02	119.91	117.40
54	1y	50	G	N1-C6-O6	-5.02	116.89	119.90
1	2A	668	G	OP2-P-O3'	5.02	116.23	105.20
1	1A	1080	C	N1-C2-O2	5.01	121.91	118.90
1	2A	2155	G	N9-C4-C5	-5.01	103.39	105.40
55	1x	46	G	N3-C2-N2	-5.01	116.39	119.90
54	2y	36	C	C5-C6-N1	5.01	123.50	121.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	14	56	VAL	Peptide
26	14	63	TYR	Peptide
26	14	64	GLY	Peptide
26	24	56	VAL	Peptide
33	2b	124	SER	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	256 (94%)	16 (6%)	1 (0%)	34	66
3	2D	273/276 (99%)	259 (95%)	13 (5%)	1 (0%)	34	66
4	1E	202/206 (98%)	194 (96%)	7 (4%)	1 (0%)	29	61
4	2E	202/206 (98%)	195 (96%)	6 (3%)	1 (0%)	29	61
5	1F	201/210 (96%)	194 (96%)	5 (2%)	2 (1%)	15	44
5	2F	201/210 (96%)	195 (97%)	4 (2%)	2 (1%)	15	44
6	1G	179/182 (98%)	168 (94%)	10 (6%)	1 (1%)	25	56
6	2G	179/182 (98%)	161 (90%)	16 (9%)	2 (1%)	14	41
7	1H	172/180 (96%)	160 (93%)	11 (6%)	1 (1%)	25	56
7	2H	172/180 (96%)	159 (92%)	10 (6%)	3 (2%)	9	29
8	1I	144/148 (97%)	127 (88%)	17 (12%)	0	100	100
8	2I	144/148 (97%)	130 (90%)	13 (9%)	1 (1%)	22	53
9	1N	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
9	2N	138/140 (99%)	133 (96%)	4 (3%)	1 (1%)	22	53
10	1O	120/122 (98%)	109 (91%)	10 (8%)	1 (1%)	19	49
10	2O	120/122 (98%)	112 (93%)	7 (6%)	1 (1%)	19	49
11	1P	147/150 (98%)	137 (93%)	9 (6%)	1 (1%)	22	53
11	2P	147/150 (98%)	138 (94%)	8 (5%)	1 (1%)	22	53
12	1Q	139/141 (99%)	133 (96%)	5 (4%)	1 (1%)	22	53
12	2Q	139/141 (99%)	130 (94%)	9 (6%)	0	100	100
13	1R	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
13	2R	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
14	1S	108/112 (96%)	99 (92%)	9 (8%)	0	100	100
14	2S	108/112 (96%)	105 (97%)	2 (2%)	1 (1%)	17	46
15	1T	129/146 (88%)	123 (95%)	6 (5%)	0	100	100
15	2T	129/146 (88%)	123 (95%)	6 (5%)	0	100	100
16	1U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
16	2U	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
17	1V	99/101 (98%)	93 (94%)	3 (3%)	3 (3%)	4	15
17	2V	99/101 (98%)	92 (93%)	5 (5%)	2 (2%)	7	24
18	1W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
18	2W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	1X	93/96 (97%)	91 (98%)	2 (2%)	0	100	100
19	2X	93/96 (97%)	90 (97%)	3 (3%)	0	100	100
20	1Y	105/110 (96%)	98 (93%)	7 (7%)	0	100	100
20	2Y	105/110 (96%)	98 (93%)	7 (7%)	0	100	100
21	1Z	148/206 (72%)	130 (88%)	16 (11%)	2 (1%)	11	34
21	2Z	156/206 (76%)	135 (86%)	19 (12%)	2 (1%)	12	36
22	10	81/85 (95%)	78 (96%)	3 (4%)	0	100	100
22	20	81/85 (95%)	80 (99%)	1 (1%)	0	100	100
23	11	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	14	41
23	21	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	14	41
24	12	68/72 (94%)	68 (100%)	0	0	100	100
24	22	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
25	13	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
25	23	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
26	14	67/71 (94%)	52 (78%)	12 (18%)	3 (4%)	2	8
26	24	67/71 (94%)	53 (79%)	10 (15%)	4 (6%)	1	4
27	15	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
27	25	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
28	16	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
28	26	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
29	17	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
29	27	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
30	18	62/65 (95%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	35 (100%)	0	0	100	100
33	1b	229/256 (90%)	201 (88%)	21 (9%)	7 (3%)	4	14
33	2b	229/256 (90%)	200 (87%)	24 (10%)	5 (2%)	6	22
34	1c	204/239 (85%)	188 (92%)	13 (6%)	3 (2%)	10	33
34	2c	204/239 (85%)	189 (93%)	14 (7%)	1 (0%)	29	61
35	1d	206/209 (99%)	195 (95%)	9 (4%)	2 (1%)	15	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
35	2d	206/209 (99%)	198 (96%)	7 (3%)	1 (0%)	29 61
36	1e	146/162 (90%)	138 (94%)	3 (2%)	5 (3%)	3 13
36	2e	146/162 (90%)	133 (91%)	12 (8%)	1 (1%)	22 53
37	1f	98/101 (97%)	94 (96%)	3 (3%)	1 (1%)	15 44
37	2f	98/101 (97%)	95 (97%)	3 (3%)	0	100 100
38	1g	153/156 (98%)	141 (92%)	9 (6%)	3 (2%)	7 24
38	2g	153/156 (98%)	145 (95%)	6 (4%)	2 (1%)	12 36
39	1h	135/138 (98%)	131 (97%)	4 (3%)	0	100 100
39	2h	135/138 (98%)	129 (96%)	6 (4%)	0	100 100
40	1i	125/128 (98%)	108 (86%)	17 (14%)	0	100 100
40	2i	125/128 (98%)	112 (90%)	13 (10%)	0	100 100
41	1j	95/105 (90%)	81 (85%)	11 (12%)	3 (3%)	4 13
41	2j	94/105 (90%)	84 (89%)	6 (6%)	4 (4%)	2 8
42	1k	112/129 (87%)	100 (89%)	10 (9%)	2 (2%)	8 28
42	2k	112/129 (87%)	99 (88%)	12 (11%)	1 (1%)	17 46
43	1l	119/132 (90%)	115 (97%)	3 (2%)	1 (1%)	19 49
43	2l	119/132 (90%)	115 (97%)	4 (3%)	0	100 100
44	1m	121/126 (96%)	110 (91%)	9 (7%)	2 (2%)	9 29
44	2m	120/126 (95%)	109 (91%)	11 (9%)	0	100 100
45	1n	58/61 (95%)	55 (95%)	3 (5%)	0	100 100
45	2n	58/61 (95%)	53 (91%)	5 (9%)	0	100 100
46	1o	86/89 (97%)	84 (98%)	2 (2%)	0	100 100
46	2o	86/89 (97%)	84 (98%)	2 (2%)	0	100 100
47	1p	80/88 (91%)	76 (95%)	4 (5%)	0	100 100
47	2p	80/88 (91%)	75 (94%)	5 (6%)	0	100 100
48	1q	97/105 (92%)	89 (92%)	8 (8%)	0	100 100
48	2q	97/105 (92%)	93 (96%)	3 (3%)	1 (1%)	15 44
49	1r	66/88 (75%)	63 (96%)	3 (4%)	0	100 100
49	2r	66/88 (75%)	63 (96%)	3 (4%)	0	100 100
50	1s	81/93 (87%)	71 (88%)	9 (11%)	1 (1%)	13 39
50	2s	81/93 (87%)	66 (82%)	13 (16%)	2 (2%)	5 19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
51	1t	94/106 (89%)	85 (90%)	6 (6%)	3 (3%)	4 13
51	2t	94/106 (89%)	86 (92%)	4 (4%)	4 (4%)	2 8
52	1u	21/27 (78%)	19 (90%)	2 (10%)	0	100 100
52	2u	21/27 (78%)	18 (86%)	1 (5%)	2 (10%)	0 1
All	All	11370/12128 (94%)	10640 (94%)	632 (6%)	98 (1%)	17 46

All (98) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
17	1V	53	GLU
33	1b	17	PHE
36	1e	98	THR
41	1j	79	ARG
50	1s	27	GLU
5	2F	130	ALA
6	2G	52	ILE
23	21	3	LYS
26	24	65	ASP
33	2b	78	GLN
51	2t	47	GLY
5	1F	89	VAL
6	1G	47	LYS
21	1Z	2	GLU
21	1Z	147	GLY
26	14	55	ARG
33	1b	13	ALA
34	1c	107	GLN
36	1e	85	GLY
43	1l	91	LYS
5	2F	89	VAL
7	2H	47	GLU
21	2Z	2	GLU
21	2Z	141	VAL
33	2b	17	PHE
36	2e	85	GLY
41	2j	75	ILE
42	2k	49	GLY
51	2t	10	LEU
52	2u	7	ARG
7	1H	126	PRO

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Mol	Chain	Res	Type
17	1V	43	GLU
26	14	58	ARG
26	14	68	ARG
33	1b	78	GLN
33	1b	125	PRO
41	1j	32	ALA
44	1m	3	ARG
51	1t	95	ALA
7	2H	126	PRO
33	2b	20	GLU
52	2u	3	LYS
17	1V	100	ARG
23	11	3	LYS
33	1b	20	GLU
33	1b	126	GLU
36	1e	86	ALA
38	1g	4	ARG
41	1j	29	ARG
51	1t	47	GLY
8	2I	42	SER
10	2O	5	GLN
17	2V	100	ARG
26	24	64	GLY
26	24	68	ARG
33	2b	9	GLU
41	2j	39	PRO
50	2s	81	ARG
51	2t	95	ALA
3	1D	3	VAL
4	1E	52	LEU
12	1Q	16	ARG
33	1b	231	GLU
34	1c	14	ILE
38	1g	52	GLU
38	1g	80	VAL
44	1m	12	ASN
3	2D	3	VAL
4	2E	52	LEU
6	2G	124	SER
9	2N	47	ALA
33	2b	36	ARG
41	2j	78	ASN

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Mol	Chain	Res	Type
41	2j	79	ARG
48	2q	99	SER
10	1O	5	GLN
36	1e	69	VAL
11	2P	122	PRO
35	2d	3	ARG
38	2g	4	ARG
34	1c	66	VAL
35	1d	5	ILE
42	1k	49	GLY
11	1P	122	PRO
14	2S	96	GLY
17	2V	79	VAL
34	2c	66	VAL
51	2t	100	ILE
35	1d	178	VAL
37	1f	40	VAL
42	1k	105	VAL
51	1t	100	ILE
7	2H	12	PRO
26	24	56	VAL
38	2g	80	VAL
50	2s	9	VAL
36	1e	70	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%)	200 (93%)	15 (7%)	15 40
3	2D	215/218 (99%)	202 (94%)	13 (6%)	19 48
4	1E	164/166 (99%)	148 (90%)	16 (10%)	8 24
4	2E	164/166 (99%)	157 (96%)	7 (4%)	29 62
5	1F	160/166 (96%)	147 (92%)	13 (8%)	11 33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	2F	159/166 (96%)	150 (94%)	9 (6%)	20 50
6	1G	143/156 (92%)	132 (92%)	11 (8%)	13 35
6	2G	143/156 (92%)	131 (92%)	12 (8%)	11 31
7	1H	144/148 (97%)	138 (96%)	6 (4%)	30 63
7	2H	144/148 (97%)	136 (94%)	8 (6%)	21 51
8	1I	113/124 (91%)	104 (92%)	9 (8%)	12 34
8	2I	105/124 (85%)	96 (91%)	9 (9%)	10 30
9	1N	118/119 (99%)	109 (92%)	9 (8%)	13 36
9	2N	118/119 (99%)	113 (96%)	5 (4%)	30 63
10	1O	100/100 (100%)	96 (96%)	4 (4%)	31 65
10	2O	100/100 (100%)	94 (94%)	6 (6%)	19 48
11	1P	115/116 (99%)	108 (94%)	7 (6%)	18 48
11	2P	115/116 (99%)	110 (96%)	5 (4%)	29 62
12	1Q	111/111 (100%)	102 (92%)	9 (8%)	11 33
12	2Q	111/111 (100%)	104 (94%)	7 (6%)	18 46
13	1R	101/101 (100%)	92 (91%)	9 (9%)	9 28
13	2R	101/101 (100%)	93 (92%)	8 (8%)	12 34
14	1S	86/88 (98%)	81 (94%)	5 (6%)	20 50
14	2S	85/88 (97%)	80 (94%)	5 (6%)	19 49
15	1T	115/127 (91%)	112 (97%)	3 (3%)	46 79
15	2T	113/127 (89%)	112 (99%)	1 (1%)	78 94
16	1U	93/94 (99%)	88 (95%)	5 (5%)	22 53
16	2U	93/94 (99%)	90 (97%)	3 (3%)	39 73
17	1V	80/82 (98%)	73 (91%)	7 (9%)	10 29
17	2V	80/82 (98%)	73 (91%)	7 (9%)	10 29
18	1W	90/92 (98%)	87 (97%)	3 (3%)	38 72
18	2W	90/92 (98%)	86 (96%)	4 (4%)	28 61
19	1X	77/78 (99%)	75 (97%)	2 (3%)	46 79
19	2X	77/78 (99%)	75 (97%)	2 (3%)	46 79
20	1Y	85/91 (93%)	80 (94%)	5 (6%)	19 49
20	2Y	85/91 (93%)	77 (91%)	8 (9%)	8 26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
21	1Z	135/179 (75%)	128 (95%)	7 (5%)	23 55
21	2Z	137/179 (76%)	129 (94%)	8 (6%)	20 50
22	10	65/67 (97%)	62 (95%)	3 (5%)	27 60
22	20	65/67 (97%)	64 (98%)	1 (2%)	65 89
23	11	80/83 (96%)	76 (95%)	4 (5%)	24 56
23	21	80/83 (96%)	75 (94%)	5 (6%)	18 46
24	12	65/67 (97%)	60 (92%)	5 (8%)	13 35
24	22	65/67 (97%)	60 (92%)	5 (8%)	13 35
25	13	51/52 (98%)	51 (100%)	0	100 100
25	23	50/52 (96%)	49 (98%)	1 (2%)	55 84
26	14	59/63 (94%)	51 (86%)	8 (14%)	3 11
26	24	53/63 (84%)	50 (94%)	3 (6%)	20 50
27	15	50/52 (96%)	46 (92%)	4 (8%)	12 34
27	25	50/52 (96%)	45 (90%)	5 (10%)	7 22
28	16	51/52 (98%)	46 (90%)	5 (10%)	8 24
28	26	50/52 (96%)	47 (94%)	3 (6%)	19 48
29	17	41/42 (98%)	38 (93%)	3 (7%)	14 38
29	27	41/42 (98%)	39 (95%)	2 (5%)	25 57
30	18	54/55 (98%)	47 (87%)	7 (13%)	4 13
30	28	54/55 (98%)	48 (89%)	6 (11%)	6 19
31	19	34/34 (100%)	33 (97%)	1 (3%)	42 76
31	29	34/34 (100%)	33 (97%)	1 (3%)	42 76
33	1b	192/220 (87%)	182 (95%)	10 (5%)	23 55
33	2b	187/220 (85%)	180 (96%)	7 (4%)	34 68
34	1c	142/188 (76%)	138 (97%)	4 (3%)	43 77
34	2c	140/188 (74%)	132 (94%)	8 (6%)	20 50
35	1d	169/181 (93%)	153 (90%)	16 (10%)	8 25
35	2d	173/181 (96%)	162 (94%)	11 (6%)	17 45
36	1e	113/123 (92%)	108 (96%)	5 (4%)	28 61
36	2e	114/123 (93%)	111 (97%)	3 (3%)	46 79
37	1f	84/90 (93%)	82 (98%)	2 (2%)	49 81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
37	2f	85/90 (94%)	81 (95%)	4 (5%)	26 59
38	1g	119/127 (94%)	116 (98%)	3 (2%)	47 80
38	2g	120/127 (94%)	119 (99%)	1 (1%)	81 94
39	1h	114/119 (96%)	104 (91%)	10 (9%)	10 29
39	2h	114/119 (96%)	109 (96%)	5 (4%)	28 61
40	1i	90/99 (91%)	86 (96%)	4 (4%)	28 61
40	2i	89/99 (90%)	82 (92%)	7 (8%)	12 34
41	1j	66/92 (72%)	63 (96%)	3 (4%)	27 60
41	2j	69/92 (75%)	67 (97%)	2 (3%)	42 76
42	1k	82/99 (83%)	81 (99%)	1 (1%)	71 92
42	2k	83/99 (84%)	79 (95%)	4 (5%)	25 58
43	1l	96/108 (89%)	89 (93%)	7 (7%)	14 38
43	2l	96/108 (89%)	89 (93%)	7 (7%)	14 38
44	1m	93/101 (92%)	89 (96%)	4 (4%)	29 62
44	2m	92/101 (91%)	86 (94%)	6 (6%)	17 44
45	1n	49/50 (98%)	43 (88%)	6 (12%)	5 15
45	2n	49/50 (98%)	47 (96%)	2 (4%)	30 64
46	1o	78/80 (98%)	76 (97%)	2 (3%)	46 79
46	2o	78/80 (98%)	77 (99%)	1 (1%)	69 91
47	1p	69/74 (93%)	62 (90%)	7 (10%)	7 22
47	2p	68/74 (92%)	62 (91%)	6 (9%)	10 29
48	1q	94/97 (97%)	94 (100%)	0	100 100
48	2q	94/97 (97%)	92 (98%)	2 (2%)	53 84
49	1r	59/77 (77%)	57 (97%)	2 (3%)	37 71
49	2r	59/77 (77%)	59 (100%)	0	100 100
50	1s	69/80 (86%)	68 (99%)	1 (1%)	67 90
50	2s	67/80 (84%)	64 (96%)	3 (4%)	27 60
51	1t	70/82 (85%)	65 (93%)	5 (7%)	14 39
51	2t	70/82 (85%)	67 (96%)	3 (4%)	29 62
52	1u	18/22 (82%)	18 (100%)	0	100 100
52	2u	18/22 (82%)	18 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9303/10064 (92%)	8785 (94%)	518 (6%)	21 51

All (518) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	32	SER
3	1D	39	LYS
3	1D	94	LEU
3	1D	113	VAL
3	1D	142	VAL
3	1D	155	LEU
3	1D	157	ARG
3	1D	173	VAL
3	1D	193	VAL
3	1D	211	ARG
3	1D	221	VAL
3	1D	229	VAL
3	1D	242	ARG
3	1D	260	ARG
3	1D	273	ARG
4	1E	1	MET
4	1E	9	VAL
4	1E	12	THR
4	1E	21	VAL
4	1E	24	THR
4	1E	27	LEU
4	1E	34	VAL
4	1E	47	VAL
4	1E	75	VAL
4	1E	82	ARG
4	1E	93	VAL
4	1E	94	GLU
4	1E	116	VAL
4	1E	145	LYS
4	1E	175	VAL
4	1E	181	LEU
5	1F	24	LEU
5	1F	32	LEU
5	1F	33	LEU
5	1F	52	LYS
5	1F	53	THR
5	1F	57	VAL

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Mol	Chain	Res	Type
5	1F	88	VAL
5	1F	106	ARG
5	1F	132	VAL
5	1F	158	THR
5	1F	183	VAL
5	1F	192	LEU
5	1F	197	ASP
6	1G	3	LEU
6	1G	5	VAL
6	1G	14	GLU
6	1G	31	VAL
6	1G	43	LEU
6	1G	82	LEU
6	1G	109	VAL
6	1G	133	LEU
6	1G	139	LEU
6	1G	149	VAL
6	1G	175	LEU
7	1H	15	VAL
7	1H	56	SER
7	1H	69	ARG
7	1H	71	LEU
7	1H	106	THR
7	1H	122	THR
8	1I	12	LEU
8	1I	31	LEU
8	1I	38	LEU
8	1I	47	LEU
8	1I	87	LYS
8	1I	92	VAL
8	1I	109	ILE
8	1I	140	LEU
8	1I	145	VAL
9	1N	28	THR
9	1N	33	LEU
9	1N	34	LEU
9	1N	35	ARG
9	1N	46	VAL
9	1N	61	ARG
9	1N	62	VAL
9	1N	87	LEU
9	1N	139	GLU

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Mol	Chain	Res	Type
10	1O	21	CYS
10	1O	69	ILE
10	1O	98	VAL
10	1O	107	ARG
11	1P	45	LEU
11	1P	56	SER
11	1P	83	VAL
11	1P	95	VAL
11	1P	125	VAL
11	1P	135	LEU
11	1P	148	LEU
12	1Q	8	LYS
12	1Q	35	VAL
12	1Q	37	LEU
12	1Q	60	ARG
12	1Q	109	VAL
12	1Q	110	THR
12	1Q	112	GLU
12	1Q	133	ARG
12	1Q	138	ASP
13	1R	6	SER
13	1R	29	LEU
13	1R	44	LEU
13	1R	54	LEU
13	1R	65	LEU
13	1R	67	LEU
13	1R	100	LEU
13	1R	111	LEU
13	1R	114	VAL
14	1S	17	ARG
14	1S	36	TYR
14	1S	50	SER
14	1S	69	VAL
14	1S	110	LEU
15	1T	28	VAL
15	1T	67	SER
15	1T	74	ARG
16	1U	5	LYS
16	1U	8	VAL
16	1U	36	ARG
16	1U	74	LEU
16	1U	95	LEU

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Mol	Chain	Res	Type
17	1V	35	LEU
17	1V	38	LEU
17	1V	46	VAL
17	1V	52	VAL
17	1V	72	VAL
17	1V	79	VAL
17	1V	82	ARG
18	1W	17	VAL
18	1W	23	LEU
18	1W	107	LEU
19	1X	38	GLU
19	1X	45	THR
20	1Y	70	SER
20	1Y	72	VAL
20	1Y	90	LEU
20	1Y	99	CYS
20	1Y	107	ASP
21	1Z	1	MET
21	1Z	8	TYR
21	1Z	28	MET
21	1Z	33	LEU
21	1Z	70	LEU
21	1Z	129	SER
21	1Z	146	ILE
22	10	14	ARG
22	10	39	ARG
22	10	43	THR
23	11	32	LYS
23	11	35	THR
23	11	59	THR
23	11	95	LEU
24	12	1	MET
24	12	19	VAL
24	12	53	LEU
24	12	62	THR
24	12	70	GLN
26	14	3	GLU
26	14	49	PHE
26	14	50	VAL
26	14	52	THR
26	14	56	VAL
26	14	58	ARG

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Mol	Chain	Res	Type
26	14	66	SER
26	14	67	TYR
27	15	6	VAL
27	15	16	ARG
27	15	29	THR
27	15	58	LEU
28	16	6	ARG
28	16	14	THR
28	16	19	ARG
28	16	24	GLU
28	16	51	GLU
29	17	1	MET
29	17	41	ARG
29	17	43	THR
30	18	14	VAL
30	18	23	VAL
30	18	30	ARG
30	18	31	HIS
30	18	32	LEU
30	18	37	SER
30	18	42	ARG
31	19	6	SER
33	1b	96	ARG
33	1b	107	THR
33	1b	111	ARG
33	1b	121	LEU
33	1b	127	ILE
33	1b	160	ASP
33	1b	189	ASP
33	1b	208	ILE
33	1b	221	LEU
33	1b	223	ILE
34	1c	15	THR
34	1c	112	SER
34	1c	115	LEU
34	1c	207	VAL
35	1d	10	ARG
35	1d	19	LEU
35	1d	31	CYS
35	1d	59	ARG
35	1d	107	ARG
35	1d	108	LEU

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Mol	Chain	Res	Type
35	1d	112	VAL
35	1d	115	ARG
35	1d	127	THR
35	1d	135	LEU
35	1d	137	SER
35	1d	144	ASP
35	1d	157	LEU
35	1d	177	ASP
35	1d	190	ASP
35	1d	194	LEU
36	1e	20	GLN
36	1e	41	VAL
36	1e	91	LEU
36	1e	116	THR
36	1e	120	THR
37	1f	2	ARG
37	1f	72	VAL
38	1g	3	ARG
38	1g	53	LYS
38	1g	79	ARG
39	1h	25	ASP
39	1h	26	VAL
39	1h	29	SER
39	1h	51	VAL
39	1h	63	LEU
39	1h	91	ARG
39	1h	95	VAL
39	1h	112	LEU
39	1h	120	THR
39	1h	133	LEU
40	1i	81	ILE
40	1i	87	GLN
40	1i	127	LYS
40	1i	128	ARG
41	1j	38	ILE
41	1j	49	VAL
41	1j	92	THR
42	1k	48	ILE
43	1l	27	LEU
43	1l	36	VAL
43	1l	54	LYS
43	1l	59	ARG

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Mol	Chain	Res	Type
43	1l	83	VAL
43	1l	113	ARG
43	1l	117	ARG
44	1m	3	ARG
44	1m	64	TRP
44	1m	102	ARG
44	1m	110	ARG
45	1n	3	ARG
45	1n	18	VAL
45	1n	22	THR
45	1n	33	VAL
45	1n	44	LEU
45	1n	60	SER
46	1o	38	ARG
46	1o	66	LEU
47	1p	2	VAL
47	1p	6	LEU
47	1p	20	VAL
47	1p	21	VAL
47	1p	25	ARG
47	1p	45	THR
47	1p	50	LYS
49	1r	35	ARG
49	1r	37	VAL
50	1s	48	THR
51	1t	8	ARG
51	1t	22	ARG
51	1t	56	MET
51	1t	70	SER
51	1t	100	ILE
3	2D	38	LYS
3	2D	61	LEU
3	2D	88	ARG
3	2D	94	LEU
3	2D	106	ILE
3	2D	116	GLN
3	2D	142	VAL
3	2D	155	LEU
3	2D	157	ARG
3	2D	212	SER
3	2D	221	VAL
3	2D	229	VAL

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Mol	Chain	Res	Type
3	2D	242	ARG
4	2E	21	VAL
4	2E	24	THR
4	2E	75	VAL
4	2E	113	PHE
4	2E	116	VAL
4	2E	175	VAL
4	2E	181	LEU
5	2F	12	LEU
5	2F	20	LEU
5	2F	30	PRO
5	2F	57	VAL
5	2F	88	VAL
5	2F	106	ARG
5	2F	169	ASN
5	2F	183	VAL
5	2F	201	VAL
6	2G	3	LEU
6	2G	5	VAL
6	2G	31	VAL
6	2G	40	ASN
6	2G	43	LEU
6	2G	88	ILE
6	2G	98	ARG
6	2G	109	VAL
6	2G	133	LEU
6	2G	140	ILE
6	2G	161	THR
6	2G	170	ARG
7	2H	15	VAL
7	2H	25	LYS
7	2H	56	SER
7	2H	63	SER
7	2H	70	THR
7	2H	107	VAL
7	2H	122	THR
7	2H	139	GLN
8	2I	20	ASP
8	2I	38	LEU
8	2I	61	ARG
8	2I	74	ASN
8	2I	77	LEU

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Mol	Chain	Res	Type
8	2I	92	VAL
8	2I	101	LEU
8	2I	127	VAL
8	2I	144	VAL
9	2N	28	THR
9	2N	33	LEU
9	2N	35	ARG
9	2N	62	VAL
9	2N	99	LEU
10	2O	21	CYS
10	2O	28	SER
10	2O	42	SER
10	2O	52	VAL
10	2O	78	ARG
10	2O	98	VAL
11	2P	3	LEU
11	2P	95	VAL
11	2P	96	THR
11	2P	106	LEU
11	2P	148	LEU
12	2Q	14	ARG
12	2Q	22	LYS
12	2Q	38	GLU
12	2Q	85	LYS
12	2Q	106	VAL
12	2Q	109	VAL
12	2Q	110	THR
13	2R	6	SER
13	2R	29	LEU
13	2R	36	THR
13	2R	44	LEU
13	2R	65	LEU
13	2R	96	ARG
13	2R	100	LEU
13	2R	111	LEU
14	2S	21	THR
14	2S	35	ILE
14	2S	36	TYR
14	2S	80	LEU
14	2S	110	LEU
15	2T	89	VAL
16	2U	5	LYS

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Mol	Chain	Res	Type
16	2U	8	VAL
16	2U	74	LEU
17	2V	7	THR
17	2V	38	LEU
17	2V	52	VAL
17	2V	61	VAL
17	2V	62	LEU
17	2V	72	VAL
17	2V	79	VAL
18	2W	23	LEU
18	2W	67	ASP
18	2W	92	ARG
18	2W	107	LEU
19	2X	57	LEU
19	2X	95	LEU
20	2Y	6	HIS
20	2Y	14	LEU
20	2Y	37	VAL
20	2Y	90	LEU
20	2Y	97	ARG
20	2Y	99	CYS
20	2Y	106	LEU
20	2Y	107	ASP
21	2Z	5	LEU
21	2Z	33	LEU
21	2Z	38	TYR
21	2Z	40	ASP
21	2Z	42	VAL
21	2Z	66	SER
21	2Z	72	ARG
21	2Z	92	SER
22	20	14	ARG
23	21	21	ARG
23	21	26	ARG
23	21	35	THR
23	21	38	SER
23	21	95	LEU
24	22	44	LEU
24	22	46	GLN
24	22	51	ARG
24	22	52	ASP
24	22	70	GLN

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Mol	Chain	Res	Type
25	23	55	ARG
26	24	1	MET
26	24	49	PHE
26	24	63	TYR
27	25	6	VAL
27	25	16	ARG
27	25	19	ARG
27	25	29	THR
27	25	58	LEU
28	26	14	THR
28	26	23	THR
28	26	51	GLU
29	27	1	MET
29	27	46	VAL
30	28	14	VAL
30	28	23	VAL
30	28	30	ARG
30	28	31	HIS
30	28	32	LEU
30	28	34	TRP
31	29	7	VAL
33	2b	67	THR
33	2b	102	LEU
33	2b	111	ARG
33	2b	160	ASP
33	2b	178	ARG
33	2b	190	THR
33	2b	230	VAL
34	2c	17	ASP
34	2c	32	LEU
34	2c	36	ASP
34	2c	49	SER
34	2c	58	GLU
34	2c	104	GLN
34	2c	115	LEU
34	2c	131	ARG
35	2d	31	CYS
35	2d	59	ARG
35	2d	83	SER
35	2d	127	THR
35	2d	135	LEU
35	2d	141	ARG

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Mol	Chain	Res	Type
35	2d	157	LEU
35	2d	176	LEU
35	2d	178	VAL
35	2d	188	LEU
35	2d	194	LEU
36	2e	41	VAL
36	2e	115	VAL
36	2e	152	ARG
37	2f	48	LEU
37	2f	55	ASP
37	2f	74	ASP
37	2f	94	GLN
38	2g	104	LEU
39	2h	25	ASP
39	2h	29	SER
39	2h	54	ASP
39	2h	87	SER
39	2h	104	ARG
40	2i	47	LEU
40	2i	87	GLN
40	2i	102	LEU
40	2i	103	THR
40	2i	111	ARG
40	2i	127	LYS
40	2i	128	ARG
41	2j	67	THR
41	2j	95	GLU
42	2k	14	VAL
42	2k	26	ASN
42	2k	48	ILE
42	2k	87	THR
43	2l	6	THR
43	2l	18	VAL
43	2l	33	ARG
43	2l	83	VAL
43	2l	113	ARG
43	2l	117	ARG
43	2l	123	LYS
44	2m	19	LEU
44	2m	49	THR
44	2m	64	TRP
44	2m	70	LEU

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Mol	Chain	Res	Type
44	2m	110	ARG
44	2m	114	ARG
45	2n	18	VAL
45	2n	33	VAL
46	2o	87	ILE
47	2p	2	VAL
47	2p	21	VAL
47	2p	60	LEU
47	2p	62	VAL
47	2p	67	THR
47	2p	69	THR
48	2q	63	ARG
48	2q	87	LYS
50	2s	27	GLU
50	2s	41	VAL
50	2s	48	THR
51	2t	22	ARG
51	2t	70	SER
51	2t	89	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (95) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	116	GLN
3	1D	126	GLN
4	1E	48	GLN
5	1F	8	GLN
5	1F	69	HIS
5	1F	203	GLN
6	1G	26	GLN
6	1G	108	ASN
8	1I	74	ASN
13	1R	71	GLN
14	1S	95	HIS
15	1T	58	ASN
16	1U	81	HIS
19	1X	31	HIS
19	1X	82	GLN
20	1Y	6	HIS
21	1Z	34	ASN
21	1Z	54	HIS
23	11	56	GLN

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Mol	Chain	Res	Type
24	12	65	ASN
25	13	32	GLN
30	18	35	GLN
31	19	34	GLN
34	1c	6	HIS
34	1c	162	GLN
35	1d	42	GLN
35	1d	77	ASN
35	1d	116	GLN
35	1d	119	GLN
35	1d	123	HIS
35	1d	161	ASN
36	1e	20	GLN
36	1e	78	HIS
37	1f	73	ASN
37	1f	100	ASN
38	1g	28	ASN
38	1g	86	GLN
38	1g	148	ASN
40	1i	3	GLN
40	1i	73	GLN
40	1i	124	GLN
41	1j	56	HIS
42	1k	38	ASN
42	1k	93	GLN
44	1m	77	ASN
44	1m	92	HIS
47	1p	13	HIS
47	1p	14	ASN
47	1p	16	HIS
48	1q	26	GLN
49	1r	63	GLN
50	1s	69	HIS
50	1s	83	HIS
51	1t	16	HIS
3	2D	87	ASN
4	2E	48	GLN
5	2F	40	GLN
5	2F	69	HIS
6	2G	66	GLN
6	2G	108	ASN
8	2I	74	ASN

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Mol	Chain	Res	Type
12	2Q	123	HIS
13	2R	13	HIS
15	2T	58	ASN
16	2U	72	HIS
19	2X	31	HIS
21	2Z	73	GLN
22	20	50	ASN
24	22	65	ASN
33	2b	78	GLN
33	2b	95	GLN
34	2c	28	GLN
34	2c	98	ASN
35	2d	77	ASN
35	2d	125	HIS
35	2d	161	ASN
36	2e	20	GLN
36	2e	78	HIS
37	2f	73	ASN
37	2f	100	ASN
38	2g	68	ASN
38	2g	86	GLN
38	2g	148	ASN
40	2i	38	GLN
40	2i	58	HIS
40	2i	87	GLN
40	2i	124	GLN
41	2j	56	HIS
42	2k	22	HIS
44	2m	12	ASN
44	2m	77	ASN
49	2r	63	GLN
50	2s	69	HIS
50	2s	83	HIS
51	2t	16	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2860/2915 (98%)	429 (15%)	28 (0%)
1	2A	2788/2915 (95%)	466 (16%)	20 (0%)
2	1B	120/121 (99%)	9 (7%)	1 (0%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	2B	119/121 (98%)	12 (10%)	1 (0%)
32	1a	1494/1521 (98%)	247 (16%)	0
32	2a	1498/1521 (98%)	282 (18%)	0
53	1v	12/27 (44%)	3 (25%)	0
53	2v	12/27 (44%)	3 (25%)	0
54	1w	68/76 (89%)	19 (27%)	0
54	1y	68/76 (89%)	30 (44%)	0
54	2w	68/76 (89%)	23 (33%)	0
54	2y	68/76 (89%)	34 (50%)	0
55	1x	75/77 (97%)	10 (13%)	0
55	2x	75/77 (97%)	11 (14%)	0
All	All	9325/9626 (96%)	1578 (16%)	50 (0%)

All (1578) 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	36	G
1	1A	45	C
1	1A	63	U
1	1A	71	A
1	1A	74	A
1	1A	75	G
1	1A	84	A
1	1A	95	G
1	1A	118	A
1	1A	119	A
1	1A	120	U
1	1A	125	G
1	1A	139(A)	G
1	1A	182	A
1	1A	196	A
1	1A	199	A
1	1A	205	G
1	1A	215	G
1	1A	216	A
1	1A	222	A
1	1A	225	A
1	1A	228	A

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Mol	Chain	Res	Type
1	1A	229	A
1	1A	230	U
1	1A	233	A
1	1A	248	G
1	1A	250	G
1	1A	266	G
1	1A	270	A
1	1A	271(K)	U
1	1A	271(L)	U
1	1A	271(M)	G
1	1A	271(N)	U
1	1A	271(O)	C
1	1A	272(A)	U
1	1A	272(B)	G
1	1A	279	C
1	1A	311	A
1	1A	324	A
1	1A	329	G
1	1A	330	A
1	1A	345	A
1	1A	352	G
1	1A	363	G
1	1A	363(B)	G
1	1A	386	G
1	1A	389	G
1	1A	396	G
1	1A	405	U
1	1A	411	G
1	1A	418	G
1	1A	421	U
1	1A	428	A
1	1A	443	A
1	1A	444	C
1	1A	448	U
1	1A	456	C
1	1A	457	A
1	1A	481	G
1	1A	504	U
1	1A	505	A
1	1A	509	C
1	1A	528	A
1	1A	529	A

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Mol	Chain	Res	Type
1	1A	530	G
1	1A	531	C
1	1A	532	A
1	1A	533	G
1	1A	545	G
1	1A	549	G
1	1A	563	G
1	1A	573	G
1	1A	575	A
1	1A	603	A
1	1A	604	G
1	1A	607	U
1	1A	614(B)	G
1	1A	614(C)	A
1	1A	615	G
1	1A	616	G
1	1A	619	G
1	1A	627	A
1	1A	637	A
1	1A	645	C
1	1A	646	A
1	1A	652(A)	A
1	1A	652(E)	G
1	1A	652(T)	C
1	1A	669	G
1	1A	677	A
1	1A	686	G
1	1A	730	C
1	1A	775	G
1	1A	776	G
1	1A	779	U
1	1A	782	A
1	1A	783	A
1	1A	784	A
1	1A	785	G
1	1A	792	G
1	1A	802	A
1	1A	805	G
1	1A	812	C
1	1A	819	A
1	1A	827	U
1	1A	828	U

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Mol	Chain	Res	Type
1	1A	859	G
1	1A	879	G
1	1A	880	G
1	1A	883	G
1	1A	884	C
1	1A	885	C
1	1A	886	C
1	1A	887	A
1	1A	888	C
1	1A	889	C
1	1A	890	A
1	1A	893	C
1	1A	894	C
1	1A	895	U
1	1A	896	A
1	1A	897	C
1	1A	898	C
1	1A	907	U
1	1A	910	A
1	1A	932	G
1	1A	945	A
1	1A	946	G
1	1A	953	A
1	1A	958	U
1	1A	959	A
1	1A	961	C
1	1A	963	U
1	1A	974	G
1	1A	975	C
1	1A	983	A
1	1A	996	A
1	1A	1012	U
1	1A	1013	C
1	1A	1025	G
1	1A	1026	U
1	1A	1033	U
1	1A	1039	G
1	1A	1041	C
1	1A	1044	G
1	1A	1046	A
1	1A	1047	G
1	1A	1054	A

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Mol	Chain	Res	Type
1	1A	1055	G
1	1A	1058	G
1	1A	1059	G
1	1A	1064	C
1	1A	1066	U
1	1A	1068	G
1	1A	1071	G
1	1A	1073	A
1	1A	1075	C
1	1A	1078	U
1	1A	1088	A
1	1A	1089	G
1	1A	1090	U
1	1A	1091	G
1	1A	1094	U
1	1A	1096	A
1	1A	1101	U
1	1A	1107	G
1	1A	1109	C
1	1A	1110	G
1	1A	1111	A
1	1A	1112	G
1	1A	1128	A
1	1A	1130	U
1	1A	1135	C
1	1A	1136	G
1	1A	1149	G
1	1A	1170	G
1	1A	1171	G
1	1A	1173	G
1	1A	1174	A
1	1A	1175	U
1	1A	1176	G
1	1A	1177	A
1	1A	1178	C
1	1A	1211	U
1	1A	1218	C
1	1A	1244	G
1	1A	1253	A
1	1A	1256	G
1	1A	1271	G
1	1A	1272	A

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Mol	Chain	Res	Type
1	1A	1273	U
1	1A	1300	U
1	1A	1301	A
1	1A	1303	G
1	1A	1352	U
1	1A	1359	A
1	1A	1360	A
1	1A	1365	A
1	1A	1372	U
1	1A	1384	A
1	1A	1385	G
1	1A	1386	C
1	1A	1396	U
1	1A	1416	G
1	1A	1417	C
1	1A	1420	U
1	1A	1421	G
1	1A	1428	C
1	1A	1437	C
1	1A	1445	A
1	1A	1450	G
1	1A	1455	G
1	1A	1467	C
1	1A	1478	G
1	1A	1482	G
1	1A	1493	C
1	1A	1494	A
1	1A	1497	U
1	1A	1508	A
1	1A	1509	C
1	1A	1509(A)	A
1	1A	1540	U
1	1A	1542	A
1	1A	1543	C
1	1A	1558	A
1	1A	1566	A
1	1A	1569	A
1	1A	1578	U
1	1A	1580	A
1	1A	1581	G
1	1A	1584	C
1	1A	1586	A

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Mol	Chain	Res	Type
1	1A	1608	A
1	1A	1609	A
1	1A	1610	A
1	1A	1648	C
1	1A	1664	A
1	1A	1674	G
1	1A	1696	G
1	1A	1700	A
1	1A	1701	A
1	1A	1703	G
1	1A	1722	A
1	1A	1746	G
1	1A	1757	U
1	1A	1758	G
1	1A	1762	A
1	1A	1763	G
1	1A	1764	G
1	1A	1773	A
1	1A	1774	C
1	1A	1780	A
1	1A	1782	C
1	1A	1791	A
1	1A	1800	C
1	1A	1801	G
1	1A	1816	G
1	1A	1829	A
1	1A	1847	A
1	1A	1861	G
1	1A	1878	G
1	1A	1889	A
1	1A	1900	A
1	1A	1906	G
1	1A	1929	G
1	1A	1930	G
1	1A	1937	A
1	1A	1938	A
1	1A	1955	U
1	1A	1963	U
1	1A	1964	G
1	1A	1967	C
1	1A	1970	A
1	1A	1971	A

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Mol	Chain	Res	Type
1	1A	1972	A
1	1A	1992	G
1	1A	1993	U
1	1A	1997	G
1	1A	2020	A
1	1A	2023	G
1	1A	2031	A
1	1A	2032	G
1	1A	2033	A
1	1A	2039	C
1	1A	2043	C
1	1A	2055	C
1	1A	2056	G
1	1A	2060	A
1	1A	2061	G
1	1A	2062	A
1	1A	2069	G
1	1A	2096	U
1	1A	2099	U
1	1A	2107	C
1	1A	2113	U
1	1A	2114	A
1	1A	2116	G
1	1A	2120	G
1	1A	2126	A
1	1A	2127	G
1	1A	2129	C
1	1A	2130	U
1	1A	2131	G
1	1A	2132	U
1	1A	2133	G
1	1A	2134	A
1	1A	2135	A
1	1A	2136	C
1	1A	2138	C
1	1A	2140	C
1	1A	2141	G
1	1A	2142	C
1	1A	2144	U
1	1A	2146	C
1	1A	2150	U
1	1A	2151	G

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Mol	Chain	Res	Type
1	1A	2155	G
1	1A	2156	G
1	1A	2157	G
1	1A	2158	A
1	1A	2159	G
1	1A	2160	G
1	1A	2163	C
1	1A	2164	C
1	1A	2165	G
1	1A	2166	G
1	1A	2167	U
1	1A	2171	A
1	1A	2172	U
1	1A	2173	A
1	1A	2174	C
1	1A	2178	C
1	1A	2181	G
1	1A	2184	G
1	1A	2193	G
1	1A	2198	A
1	1A	2206	G
1	1A	2207	G
1	1A	2208	A
1	1A	2218	U
1	1A	2225	A
1	1A	2238	G
1	1A	2268	A
1	1A	2269	A
1	1A	2273	A
1	1A	2283	C
1	1A	2287	A
1	1A	2305	A
1	1A	2308	G
1	1A	2312	U
1	1A	2320	A
1	1A	2325	G
1	1A	2334	G
1	1A	2335	A
1	1A	2336	A
1	1A	2347	C
1	1A	2350	C
1	1A	2361	A

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Mol	Chain	Res	Type
1	1A	2372	G
1	1A	2383	G
1	1A	2385	C
1	1A	2406	U
1	1A	2425	A
1	1A	2429	G
1	1A	2430	A
1	1A	2434	A
1	1A	2435	A
1	1A	2439	A
1	1A	2441	C
1	1A	2448	A
1	1A	2476	A
1	1A	2478	A
1	1A	2490	G
1	1A	2494	G
1	1A	2502	G
1	1A	2505	G
1	1A	2506	U
1	1A	2518	A
1	1A	2520	C
1	1A	2529	G
1	1A	2554	U
1	1A	2566	A
1	1A	2567	G
1	1A	2573	C
1	1A	2582	G
1	1A	2602	A
1	1A	2609	U
1	1A	2611	U
1	1A	2612	C
1	1A	2629	A
1	1A	2630	G
1	1A	2654	A
1	1A	2689	U
1	1A	2701	C
1	1A	2702	U
1	1A	2703	C
1	1A	2712(A)	A
1	1A	2713	A
1	1A	2714	G
1	1A	2726	U

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Mol	Chain	Res	Type
1	1A	2733	A
1	1A	2757	A
1	1A	2761	G
1	1A	2764	A
1	1A	2765	A
1	1A	2769	C
1	1A	2778	A
1	1A	2789	C
1	1A	2790	A
1	1A	2791	C
1	1A	2794	C
1	1A	2802	G
1	1A	2805	G
1	1A	2818	G
1	1A	2820	A
1	1A	2821	A
1	1A	2832	U
1	1A	2833	G
1	1A	2835	A
1	1A	2872	G
1	1A	2873	A
1	1A	2880	C
1	1A	2883	A
1	1A	2892	A
1	1A	2894	G
1	2A	10	G
1	2A	11	G
1	2A	15	G
1	2A	34	C
1	2A	35	G
1	2A	45	C
1	2A	55	G
1	2A	59	U
1	2A	61	G
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	84	A
1	2A	90	U
1	2A	94	C
1	2A	95	G
1	2A	100	G

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Mol	Chain	Res	Type
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	141	A
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	222	A
1	2A	228	A
1	2A	229	A
1	2A	230	U
1	2A	233	A
1	2A	248	G
1	2A	249	C
1	2A	250	G
1	2A	266	G
1	2A	271(J)	C
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	277	C
1	2A	278	A
1	2A	311	A
1	2A	317	G
1	2A	327	G
1	2A	329	G
1	2A	330	A
1	2A	332	A
1	2A	352	G

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Mol	Chain	Res	Type
1	2A	354	G
1	2A	363(B)	G
1	2A	386	G
1	2A	396	G
1	2A	411	G
1	2A	412	A
1	2A	422	A
1	2A	443	A
1	2A	444	C
1	2A	454	A
1	2A	455	C
1	2A	457	A
1	2A	480	A
1	2A	481	G
1	2A	505	A
1	2A	508	G
1	2A	509	C
1	2A	529	A
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	533	G
1	2A	556	G
1	2A	563	G
1	2A	568	U
1	2A	573	G
1	2A	575	A
1	2A	599	G
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	614(B)	G
1	2A	614(C)	A
1	2A	615	G
1	2A	616	G
1	2A	627	A
1	2A	634	C
1	2A	637	A
1	2A	645	C
1	2A	646	A
1	2A	651	G
1	2A	652(B)	A

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Mol	Chain	Res	Type
1	2A	652(C)	G
1	2A	653	A
1	2A	668	G
1	2A	669	G
1	2A	686	G
1	2A	717	G
1	2A	730	C
1	2A	752	A
1	2A	753	C
1	2A	771	G
1	2A	775	G
1	2A	776	G
1	2A	782	A
1	2A	784	A
1	2A	785	G
1	2A	790	C
1	2A	792	G
1	2A	805	G
1	2A	812	C
1	2A	819	A
1	2A	827	U
1	2A	832	G
1	2A	857	C
1	2A	859	G
1	2A	866	A
1	2A	869	G
1	2A	875	G
1	2A	878	A
1	2A	879	G
1	2A	881	G
1	2A	884	C
1	2A	886	C
1	2A	887	A
1	2A	888	C
1	2A	889	C
1	2A	893	C
1	2A	894	C
1	2A	895	U
1	2A	896	A
1	2A	900	A
1	2A	901	A
1	2A	910	A

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Mol	Chain	Res	Type
1	2A	917	A
1	2A	932	G
1	2A	933	A
1	2A	938	G
1	2A	941	A
1	2A	945	A
1	2A	946	G
1	2A	953	A
1	2A	958	U
1	2A	959	A
1	2A	961	C
1	2A	974	G
1	2A	975	C
1	2A	980	A
1	2A	983	A
1	2A	996	A
1	2A	1003	G
1	2A	1012	U
1	2A	1013	C
1	2A	1017	G
1	2A	1022	G
1	2A	1023	U
1	2A	1025	G
1	2A	1033	U
1	2A	1038	C
1	2A	1043	C
1	2A	1114	G
1	2A	1117	G
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1139	G
1	2A	1142(A)	A
1	2A	1167	U
1	2A	1170	G
1	2A	1171	G
1	2A	1188	U
1	2A	1210	A
1	2A	1211	U
1	2A	1220	A
1	2A	1253	A
1	2A	1256	G

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Mol	Chain	Res	Type
1	2A	1271	G
1	2A	1272	A
1	2A	1273	U
1	2A	1300	U
1	2A	1301	A
1	2A	1303	G
1	2A	1314	C
1	2A	1342	A
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	1380	G
1	2A	1384	A
1	2A	1385	G
1	2A	1386	C
1	2A	1395	A
1	2A	1416	G
1	2A	1417	C
1	2A	1420	U
1	2A	1421	G
1	2A	1427	A
1	2A	1428	C
1	2A	1437	C
1	2A	1445	A
1	2A	1449	A
1	2A	1450	G
1	2A	1461	G
1	2A	1467	C
1	2A	1471	A
1	2A	1482	G
1	2A	1490	A
1	2A	1493	C
1	2A	1494	A
1	2A	1496	A
1	2A	1497	U
1	2A	1506	C
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1525	G

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Mol	Chain	Res	Type
1	2A	1531	C
1	2A	1532	C
1	2A	1545	A
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	1584	C
1	2A	1586	A
1	2A	1608	A
1	2A	1609	A
1	2A	1610	A
1	2A	1634	A
1	2A	1639	U
1	2A	1647	G
1	2A	1648	C
1	2A	1654	A
1	2A	1664	A
1	2A	1667	G
1	2A	1674	G
1	2A	1696	G
1	2A	1700	A
1	2A	1701	A
1	2A	1703	G
1	2A	1721	G
1	2A	1722	A
1	2A	1740	G
1	2A	1746	G
1	2A	1756	G
1	2A	1762	A
1	2A	1763	G
1	2A	1764	G
1	2A	1773	A
1	2A	1780	A
1	2A	1782	C
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1812	A
1	2A	1816	G

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Mol	Chain	Res	Type
1	2A	1820	U
1	2A	1847	A
1	2A	1848	A
1	2A	1858	G
1	2A	1877	A
1	2A	1878	G
1	2A	1900	A
1	2A	1906	G
1	2A	1913	A
1	2A	1914	C
1	2A	1929	G
1	2A	1930	G
1	2A	1936	A
1	2A	1938	A
1	2A	1955	U
1	2A	1963	U
1	2A	1966	A
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1984	G
1	2A	1992	G
1	2A	1993	U
1	2A	1997	G
1	2A	2023	G
1	2A	2031	A
1	2A	2032	G
1	2A	2033	A
1	2A	2036	C
1	2A	2043	C
1	2A	2055	C
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G
1	2A	2069	G
1	2A	2093	G
1	2A	2099	U
1	2A	2106	G
1	2A	2108	C
1	2A	2109	U
1	2A	2110	G

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Mol	Chain	Res	Type
1	2A	2111	C
1	2A	2115	G
1	2A	2116	G
1	2A	2117	A
1	2A	2119	A
1	2A	2120	G
1	2A	2122	U
1	2A	2124	G
1	2A	2125	G
1	2A	2126	A
1	2A	2127	G
1	2A	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	2141	G
1	2A	2143	C
1	2A	2146	C
1	2A	2150	U
1	2A	2153	G
1	2A	2154	G
1	2A	2155	G
1	2A	2156	G
1	2A	2157	G
1	2A	2158	A
1	2A	2160	G
1	2A	2162	G
1	2A	2164	C
1	2A	2165	G
1	2A	2167	U
1	2A	2168	G
1	2A	2169	A
1	2A	2170	A
1	2A	2172	U
1	2A	2173	A
1	2A	2174	C

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Mol	Chain	Res	Type
1	2A	2182	G
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	2235	G
1	2A	2238	G
1	2A	2239	G
1	2A	2248	C
1	2A	2268	A
1	2A	2273	A
1	2A	2275	C
1	2A	2279	G
1	2A	2283	C
1	2A	2287	A
1	2A	2288	A
1	2A	2294	C
1	2A	2304	G
1	2A	2305	A
1	2A	2307	G
1	2A	2308	G
1	2A	2312	U
1	2A	2319	G
1	2A	2320	A
1	2A	2325	G
1	2A	2334	G
1	2A	2336	A
1	2A	2343	C
1	2A	2346	A
1	2A	2347	C
1	2A	2350	C
1	2A	2354	G
1	2A	2376	A
1	2A	2379	G
1	2A	2383	G
1	2A	2385	C
1	2A	2402	C
1	2A	2403	C

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Mol	Chain	Res	Type
1	2A	2406	U
1	2A	2425	A
1	2A	2428	G
1	2A	2429	G
1	2A	2430	A
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2448	A
1	2A	2469	A
1	2A	2474	C
1	2A	2476	A
1	2A	2490	G
1	2A	2494	G
1	2A	2497	A
1	2A	2502	G
1	2A	2504	U
1	2A	2505	G
1	2A	2506	U
1	2A	2518	A
1	2A	2520	C
1	2A	2525	G
1	2A	2536	G
1	2A	2554	U
1	2A	2566	A
1	2A	2567	G
1	2A	2573	C
1	2A	2582	G
1	2A	2585	U
1	2A	2602	A
1	2A	2611	U
1	2A	2612	C
1	2A	2630	G
1	2A	2632	A
1	2A	2634	G
1	2A	2654	A
1	2A	2669	G
1	2A	2689	U
1	2A	2690	C
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G

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Mol	Chain	Res	Type
1	2A	2718	G
1	2A	2726	U
1	2A	2733	A
1	2A	2744	G
1	2A	2748	A
1	2A	2751	G
1	2A	2757	A
1	2A	2759	G
1	2A	2761	G
1	2A	2764	A
1	2A	2765	A
1	2A	2766	G
1	2A	2778	A
1	2A	2793	G
1	2A	2794	C
1	2A	2818	G
1	2A	2820	A
1	2A	2821	A
1	2A	2835	A
1	2A	2865	U
1	2A	2866	U
1	2A	2872	G
1	2A	2879	C
1	2A	2880	C
1	2A	2886	G
1	2A	2892	A
1	2A	2894	G
1	2A	2895	U
1	2A	2897	U
2	1B	2	C
2	1B	13	A
2	1B	42	C
2	1B	52	A
2	1B	56	G
2	1B	73	A
2	1B	106	G
2	1B	110	G
2	1B	120	A
32	1a	7	G
32	1a	9	G
32	1a	32	A
32	1a	39	G

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Mol	Chain	Res	Type
32	1a	47	C
32	1a	48	C
32	1a	51	A
32	1a	52	G
32	1a	61	G
32	1a	73	G
32	1a	78	G
32	1a	79	G
32	1a	98	G
32	1a	101	A
32	1a	105	G
32	1a	116	A
32	1a	121	C
32	1a	131	C
32	1a	143	A
32	1a	162	A
32	1a	163	C
32	1a	174	C
32	1a	180	U
32	1a	183	G
32	1a	189(F)	U
32	1a	189(G)	G
32	1a	189(H)	G
32	1a	189(J)	G
32	1a	195	A
32	1a	197	A
32	1a	201	C
32	1a	202	U
32	1a	203	U
32	1a	204	U
32	1a	216	G
32	1a	247	G
32	1a	251	G
32	1a	266	G
32	1a	267	C
32	1a	289	G
32	1a	301	G
32	1a	321	A
32	1a	328	C
32	1a	332	G
32	1a	342	C
32	1a	345	C

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Mol	Chain	Res	Type
32	1a	346	G
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	384	G
32	1a	392	G
32	1a	397	A
32	1a	398	C
32	1a	406	G
32	1a	412	A
32	1a	421	U
32	1a	422	C
32	1a	424	G
32	1a	429	U
32	1a	439	A
32	1a	442	C
32	1a	452	A
32	1a	457	C
32	1a	458	C
32	1a	461	A
32	1a	470	C
32	1a	485	G
32	1a	496	A
32	1a	498	U
32	1a	508	C
32	1a	510	A
32	1a	511	C
32	1a	518	C
32	1a	519	C
32	1a	531	U
32	1a	532	A
32	1a	536	C
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

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Mol	Chain	Res	Type
32	1a	576	G
32	1a	577	G
32	1a	596	C
32	1a	619	U
32	1a	630	G
32	1a	631	G
32	1a	653	A
32	1a	661	G
32	1a	665	A
32	1a	680	C
32	1a	687	A
32	1a	688	G
32	1a	717	C
32	1a	723	U
32	1a	724	G
32	1a	734	G
32	1a	749	C
32	1a	755	G
32	1a	766	A
32	1a	774	G
32	1a	777	A
32	1a	792	A
32	1a	793	U
32	1a	794	A
32	1a	816	A
32	1a	817	C
32	1a	821	G
32	1a	828	A
32	1a	840	C
32	1a	841	U
32	1a	851	G
32	1a	859	A
32	1a	870	U
32	1a	873	A
32	1a	876	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	939	G

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Mol	Chain	Res	Type
32	1a	960	U
32	1a	961	U
32	1a	964	A
32	1a	966	M2G
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	974	A
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	992	U
32	1a	993	G
32	1a	994	A
32	1a	997	U
32	1a	1000	U
32	1a	1001(A)	G
32	1a	1003	G
32	1a	1005	A
32	1a	1006	C
32	1a	1008	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	1028	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	1044	A
32	1a	1054	C
32	1a	1055	A
32	1a	1056	U
32	1a	1065	U
32	1a	1066	C
32	1a	1068	G
32	1a	1070	U

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Mol	Chain	Res	Type
32	1a	1081	G
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1108	G
32	1a	1124	G
32	1a	1125	U
32	1a	1131	G
32	1a	1132	C
32	1a	1134	G
32	1a	1137	C
32	1a	1138	G
32	1a	1139	G
32	1a	1141	C
32	1a	1146	A
32	1a	1152	A
32	1a	1157	A
32	1a	1159	U
32	1a	1160	G
32	1a	1184	G
32	1a	1196	U
32	1a	1197	G
32	1a	1202	G
32	1a	1204	A
32	1a	1212	U
32	1a	1213	A
32	1a	1214	C
32	1a	1227	A
32	1a	1229	A
32	1a	1236	A
32	1a	1238	A
32	1a	1256	A
32	1a	1257	U
32	1a	1260	C
32	1a	1273	G
32	1a	1275	A
32	1a	1276	G
32	1a	1278	U
32	1a	1279	A
32	1a	1280	A
32	1a	1286	A
32	1a	1287	A

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Mol	Chain	Res	Type
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1305	G
32	1a	1320	C
32	1a	1338	G
32	1a	1346	A
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1364	U
32	1a	1370	G
32	1a	1378	C
32	1a	1396	A
32	1a	1397	C
32	1a	1419	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1442(B)	A
32	1a	1446	U
32	1a	1447	A
32	1a	1452	C
32	1a	1456	G
32	1a	1487	G
32	1a	1492	A
32	1a	1497	G
32	1a	1503	A
32	1a	1504	G
32	1a	1506	U
32	1a	1507	A
32	1a	1517	G
32	1a	1529	G
32	1a	1530	G
53	1v	13	A
53	1v	14	A
53	1v	24	C
54	1w	2	G
54	1w	7	U
54	1w	9	A
54	1w	19	G
54	1w	24	G
54	1w	42	G

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Mol	Chain	Res	Type
54	1w	45	G
54	1w	46	7MG
54	1w	47	U
54	1w	49	G
54	1w	50	G
54	1w	51	C
54	1w	56	C
54	1w	58	A
54	1w	61	C
54	1w	62	C
54	1w	68	C
54	1w	70	C
54	1w	74	C
55	1x	9	G
55	1x	13	C
55	1x	18	G
55	1x	19	G
55	1x	20	U
55	1x	21	A
55	1x	22	G
55	1x	47	U
55	1x	61	C
55	1x	76	A
54	1y	2	G
54	1y	5	G
54	1y	6	A
54	1y	7	U
54	1y	9	A
54	1y	10	G
54	1y	13	C
54	1y	19	G
54	1y	23	A
54	1y	24	G
54	1y	26	A
54	1y	31	C
54	1y	35	A
54	1y	36	C
54	1y	40	G
54	1y	44	G
54	1y	45	G
54	1y	46	7MG
54	1y	48	C

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Mol	Chain	Res	Type
54	1y	49	G
54	1y	54	5MU
54	1y	56	C
54	1y	57	G
54	1y	58	A
54	1y	59	U
54	1y	61	C
54	1y	64	U
54	1y	65	C
54	1y	69	A
54	1y	70	C
2	2B	2	C
2	2B	13	A
2	2B	25	A
2	2B	30	C
2	2B	33	G
2	2B	34	U
2	2B	42	C
2	2B	56	G
2	2B	58	A
2	2B	73	A
2	2B	85	G
2	2B	110	G
32	2a	7	G
32	2a	8	A
32	2a	9	G
32	2a	22	G
32	2a	32	A
32	2a	39	G
32	2a	41	G
32	2a	47	C
32	2a	48	C
32	2a	50	A
32	2a	51	A
32	2a	52	G
32	2a	66	G
32	2a	73	G
32	2a	88	A
32	2a	89	C
32	2a	101	A
32	2a	116	A
32	2a	121	C

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Mol	Chain	Res	Type
32	2a	129(A)	G
32	2a	131	C
32	2a	142	G
32	2a	144	G
32	2a	146	G
32	2a	156	G
32	2a	159	G
32	2a	163	C
32	2a	170	U
32	2a	174	C
32	2a	182	U
32	2a	189(F)	U
32	2a	189(J)	G
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	266	G
32	2a	267	C
32	2a	279	A
32	2a	289	G
32	2a	306	G
32	2a	316	G
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	342	C
32	2a	346	G
32	2a	351	G
32	2a	352	C
32	2a	353	A
32	2a	354	G
32	2a	367	U
32	2a	372	C
32	2a	373	A
32	2a	397	A
32	2a	398	C

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Mol	Chain	Res	Type
32	2a	406	G
32	2a	412	A
32	2a	421	U
32	2a	429	U
32	2a	430	A
32	2a	439	A
32	2a	442	C
32	2a	452	A
32	2a	470	C
32	2a	484	G
32	2a	485	G
32	2a	496	A
32	2a	498	U
32	2a	505	G
32	2a	506	G
32	2a	509	A
32	2a	510	A
32	2a	511	C
32	2a	518	C
32	2a	521	G
32	2a	524	G
32	2a	527	7MG
32	2a	531	U
32	2a	532	A
32	2a	533	A
32	2a	547	A
32	2a	559	A
32	2a	560	U
32	2a	561	U
32	2a	564	C
32	2a	568	G
32	2a	572	A
32	2a	573	A
32	2a	574	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

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Mol	Chain	Res	Type
32	2a	665	A
32	2a	666	G
32	2a	687	A
32	2a	688	G
32	2a	695	A
32	2a	723	U
32	2a	729	A
32	2a	731	G
32	2a	733	A
32	2a	734	G
32	2a	746	A
32	2a	749	C
32	2a	755	G
32	2a	763	G
32	2a	777	A
32	2a	792	A
32	2a	793	U
32	2a	794	A
32	2a	805	C
32	2a	815	A
32	2a	816	A
32	2a	817	C
32	2a	821	G
32	2a	828	A
32	2a	840	C
32	2a	841	U
32	2a	851	G
32	2a	853	G
32	2a	859	A
32	2a	873	A
32	2a	891	U
32	2a	902	G
32	2a	914	A
32	2a	916	G
32	2a	926	G
32	2a	927	G
32	2a	931	C
32	2a	933	G
32	2a	934	C
32	2a	935	A
32	2a	960	U
32	2a	961	U

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Mol	Chain	Res	Type
32	2a	968	A
32	2a	969	A
32	2a	971	G
32	2a	974	A
32	2a	975	A
32	2a	976	G
32	2a	977	A
32	2a	982	U
32	2a	983	A
32	2a	984	C
32	2a	992	U
32	2a	993	G
32	2a	994	A
32	2a	997	U
32	2a	998	G
32	2a	999	C
32	2a	1001(A)	G
32	2a	1002	G
32	2a	1003	G
32	2a	1004	A
32	2a	1005	A
32	2a	1006	C
32	2a	1009	G
32	2a	1020	U
32	2a	1022	G
32	2a	1023	G
32	2a	1024	G
32	2a	1026	G
32	2a	1027	C
32	2a	1028	C
32	2a	1030(A)	G
32	2a	1030(C)	G
32	2a	1036	G
32	2a	1037	C
32	2a	1039	C
32	2a	1040	U
32	2a	1045	C
32	2a	1046	A
32	2a	1053	G
32	2a	1056	U
32	2a	1064	G
32	2a	1065	U

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Mol	Chain	Res	Type
32	2a	1066	C
32	2a	1068	G
32	2a	1077	G
32	2a	1081	G
32	2a	1085	U
32	2a	1086	U
32	2a	1094	G
32	2a	1095	U
32	2a	1101	A
32	2a	1103	C
32	2a	1108	G
32	2a	1117	G
32	2a	1118	C
32	2a	1122	U
32	2a	1125	U
32	2a	1129	C
32	2a	1130	A
32	2a	1132	C
32	2a	1136	U
32	2a	1138	G
32	2a	1139	G
32	2a	1141	C
32	2a	1146	A
32	2a	1152	A
32	2a	1157	A
32	2a	1159	U
32	2a	1181	G
32	2a	1182	G
32	2a	1183	A
32	2a	1184	G
32	2a	1196	U
32	2a	1197	G
32	2a	1202	G
32	2a	1204	A
32	2a	1207	2MG
32	2a	1208	C
32	2a	1210	C
32	2a	1211	U
32	2a	1212	U
32	2a	1213	A
32	2a	1214	C
32	2a	1220	G

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Mol	Chain	Res	Type
32	2a	1222	G
32	2a	1227	A
32	2a	1238	A
32	2a	1240	U
32	2a	1241	G
32	2a	1256	A
32	2a	1257	U
32	2a	1258	G
32	2a	1260	C
32	2a	1270	C
32	2a	1272	G
32	2a	1273	G
32	2a	1275	A
32	2a	1277	C
32	2a	1278	U
32	2a	1279	A
32	2a	1280	A
32	2a	1281	U
32	2a	1282	C
32	2a	1286	A
32	2a	1287	A
32	2a	1293	G
32	2a	1294	G
32	2a	1299	A
32	2a	1302	U
32	2a	1303	C
32	2a	1305	G
32	2a	1320	C
32	2a	1340	A
32	2a	1346	A
32	2a	1347	G
32	2a	1353	G
32	2a	1363	C
32	2a	1368	G
32	2a	1370	G
32	2a	1397	C
32	2a	1404	5MC
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1446	U
32	2a	1447	A

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Mol	Chain	Res	Type
32	2a	1452	C
32	2a	1456	G
32	2a	1492	A
32	2a	1493	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
32	2a	1530	G
53	2v	13	A
53	2v	14	A
53	2v	24	C
54	2w	2	G
54	2w	7	U
54	2w	9	A
54	2w	19	G
54	2w	22	G
54	2w	24	G
54	2w	40	G
54	2w	43	G
54	2w	46	7MG
54	2w	47	U
54	2w	48	C
54	2w	49	G
54	2w	50	G
54	2w	51	C
54	2w	56	C
54	2w	57	G
54	2w	58	A
54	2w	59	U
54	2w	60	C
54	2w	62	C
54	2w	68	C
54	2w	70	C
54	2w	74	C
55	2x	9	G
55	2x	13	C
55	2x	18	G
55	2x	19	G
55	2x	20	U

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Mol	Chain	Res	Type
55	2x	21	A
55	2x	47	U
55	2x	48	C
55	2x	56	C
55	2x	61	C
55	2x	76	A
54	2y	2	G
54	2y	3	G
54	2y	5	G
54	2y	6	A
54	2y	7	U
54	2y	8	4SU
54	2y	9	A
54	2y	11	C
54	2y	13	C
54	2y	14	A
54	2y	15	G
54	2y	19	G
54	2y	22	G
54	2y	24	G
54	2y	26	A
54	2y	35	A
54	2y	38	A
54	2y	40	G
54	2y	41	A
54	2y	43	G
54	2y	47	U
54	2y	49	G
54	2y	51	C
54	2y	52	G
54	2y	53	G
54	2y	57	G
54	2y	58	A
54	2y	59	U
54	2y	61	C
54	2y	62	C
54	2y	66	A
54	2y	69	A
54	2y	70	C
54	2y	73	A

All (50) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	196	A
1	1A	266	G
1	1A	271(K)	U
1	1A	278	A
1	1A	746	A
1	1A	764	A
1	1A	774	A
1	1A	895	U
1	1A	974	G
1	1A	1065	U
1	1A	1067	A
1	1A	1142(A)	A
1	1A	1174	A
1	1A	1175	U
1	1A	1176	G
1	1A	1210	A
1	1A	1442	G
1	1A	1508	A
1	1A	1608	A
1	1A	1992	G
1	1A	2134	A
1	1A	2170	A
1	1A	2183	C
1	1A	2238	G
1	1A	2406	U
1	1A	2430	A
1	1A	2439	A
1	1A	2756	U
1	2A	228	A
1	2A	266	G
1	2A	271(M)	G
1	2A	277	C
1	2A	479	A
1	2A	528	A
1	2A	752	A
1	2A	827	U
1	2A	856	C
1	2A	893	C
1	2A	900	A
1	2A	1210	A
1	2A	1379	A
1	2A	1420	U
1	2A	1442	G

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Mol	Chain	Res	Type
1	2A	1608	A
1	2A	1913	A
1	2A	1992	G
1	2A	2689	U
1	2A	2756	U
2	1B	1	U
2	2B	1	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
32	5MC	1a	1407	32	18,22,23	0.91	2 (11%)	26,32,35	1.10	2 (7%)
1	5MC	1A	1962	56,1	18,22,23	0.91	2 (11%)	26,32,35	1.17	1 (3%)
32	MA6	2a	1519	32	19,26,27	1.03	1 (5%)	18,38,41	1.57	4 (22%)
54	5MU	1w	54	54	19,22,23	1.46	6 (31%)	28,32,35	2.34	6 (21%)
54	6MZ	1w	37	54	18,25,26	0.93	1 (5%)	16,36,39	2.10	4 (25%)
1	4OC	1A	1920	1	19,22,24	0.78	0	26,31,35	0.93	1 (3%)
32	UR3	2a	1498	32	19,22,23	1.04	1 (5%)	26,32,35	1.46	2 (7%)
1	5MU	2A	1939	1	19,22,23	1.45	5 (26%)	28,32,35	2.29	7 (25%)
1	PSU	1A	2605	56,1	18,21,22	1.36	3 (16%)	22,30,33	1.94	4 (18%)
55	5MC	2x	32	55	18,22,23	1.00	2 (11%)	26,32,35	1.29	3 (11%)
54	4SU	1y	8	54	18,21,22	1.72	5 (27%)	26,30,33	1.95	5 (19%)
1	OMG	2A	2251	56,1,55	18,26,27	0.98	1 (5%)	19,38,41	1.14	3 (15%)
43	0TD	2l	92	43	7,9,10	4.80	1 (14%)	6,11,13	2.69	3 (50%)
1	5MU	1A	1915	1	19,22,23	1.44	5 (26%)	28,32,35	2.09	7 (25%)
32	4OC	1a	1402	56,32	20,23,24	0.73	0	26,32,35	1.02	1 (3%)
32	UR3	1a	1498	32	19,22,23	1.11	1 (5%)	26,32,35	1.47	3 (11%)
54	7MG	2w	46	54	22,26,27	1.34	4 (18%)	29,39,42	2.55	7 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
54	CM0	1w	34	54	22,26,27	1.55	3 (13%)	28,37,40	1.63	4 (14%)
54	5MU	1y	54	54	19,22,23	1.42	5 (26%)	28,32,35	2.04	6 (21%)
32	MA6	2a	1518	32	19,26,27	1.05	1 (5%)	18,38,41	1.66	4 (22%)
54	CM0	2w	34	54	22,26,27	1.55	3 (13%)	28,37,40	1.67	4 (14%)
32	2MG	2a	1207	56,32	18,26,27	0.91	1 (5%)	16,38,41	1.02	1 (6%)
1	2MA	2A	2503	1	17,25,26	1.07	1 (5%)	17,37,40	0.92	2 (11%)
32	7MG	2a	527	56,32	22,26,27	1.40	4 (18%)	29,39,42	2.40	6 (20%)
1	PSU	1A	1917	1	18,21,22	1.39	2 (11%)	22,30,33	1.87	3 (13%)
54	4SU	1w	8	54	18,21,22	1.68	5 (27%)	26,30,33	1.97	4 (15%)
54	7MG	1w	46	54	22,26,27	1.37	3 (13%)	29,39,42	2.47	6 (20%)
32	M2G	1a	966	32	20,27,28	1.43	3 (15%)	22,40,43	0.95	2 (9%)
1	PSU	2A	1911	1	18,21,22	1.37	2 (11%)	22,30,33	1.82	3 (13%)
55	5MU	1x	54	56,55	19,22,23	1.41	5 (26%)	28,32,35	1.96	6 (21%)
32	7MG	1a	527	56,32	22,26,27	1.38	4 (18%)	29,39,42	2.45	7 (24%)
54	4SU	2y	8	54	18,21,22	1.71	4 (22%)	26,30,33	2.32	6 (23%)
43	0TD	1l	92	43	7,9,10	4.87	1 (14%)	6,11,13	4.10	3 (50%)
32	5MC	2a	1404	32	18,22,23	0.95	2 (11%)	26,32,35	1.16	3 (11%)
54	7MG	1y	46	54	22,26,27	1.40	3 (13%)	29,39,42	2.64	7 (24%)
54	CM0	1y	34	54	22,26,27	1.74	3 (13%)	28,37,40	2.01	4 (14%)
32	5MC	1a	1400	32	18,22,23	0.94	2 (11%)	26,32,35	1.16	2 (7%)
1	PSU	2A	2605	1	18,21,22	1.36	3 (16%)	22,30,33	1.95	4 (18%)
1	OMG	1A	2251	56,1,55	18,26,27	1.05	1 (5%)	19,38,41	1.15	2 (10%)
32	5MC	2a	1400	32	18,22,23	0.94	2 (11%)	26,32,35	1.18	2 (7%)
1	5MU	1A	1939	1	19,22,23	1.41	5 (26%)	28,32,35	2.19	6 (21%)
55	4SU	2x	8	55	18,21,22	1.95	4 (22%)	26,30,33	1.41	5 (19%)
54	6MZ	2w	37	54	18,25,26	0.92	1 (5%)	16,36,39	2.02	4 (25%)
1	5MC	1A	1942	1	18,22,23	0.93	2 (11%)	26,32,35	1.16	2 (7%)
32	2MG	1a	1207	32	18,26,27	0.97	1 (5%)	16,38,41	1.07	1 (6%)
54	PSU	1y	55	54	18,21,22	1.33	2 (11%)	22,30,33	1.98	4 (18%)
55	PSU	2x	55	55	18,21,22	1.33	2 (11%)	22,30,33	1.84	4 (18%)
1	4OC	2A	1920	1	19,22,24	0.84	0	26,31,35	0.97	1 (3%)
1	5MC	2A	1962	56,1	18,22,23	0.96	2 (11%)	26,32,35	1.16	2 (7%)
1	2MU	1A	2552	56,1	19,22,24	1.22	2 (10%)	26,31,36	1.97	6 (23%)
32	MA6	1a	1518	32	19,26,27	0.99	1 (5%)	18,38,41	1.66	6 (33%)
32	5MC	2a	1407	56,32	18,22,23	0.97	2 (11%)	26,32,35	1.16	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	M2G	2a	966	32	20,27,28	1.52	3 (15%)	22,40,43	0.93	2 (9%)
54	5MU	2w	54	54	19,22,23	1.40	4 (21%)	28,32,35	1.92	6 (21%)
1	5MU	2A	1915	1	19,22,23	1.47	5 (26%)	28,32,35	2.16	6 (21%)
32	4OC	2a	1402	56,32	20,23,24	0.74	0	26,32,35	1.02	2 (7%)
1	5MC	2A	1942	1	18,22,23	0.97	2 (11%)	26,32,35	1.13	2 (7%)
32	5MC	1a	967	32	18,22,23	0.92	2 (11%)	26,32,35	1.09	2 (7%)
54	PSU	2y	55	54	18,21,22	1.34	2 (11%)	22,30,33	1.83	3 (13%)
32	MA6	1a	1519	32	19,26,27	1.05	1 (5%)	18,38,41	1.64	4 (22%)
54	6MZ	1y	37	54	18,25,26	1.04	2 (11%)	16,36,39	2.19	4 (25%)
54	CM0	2y	34	53,54	22,26,27	1.58	2 (9%)	28,37,40	1.94	4 (14%)
54	PSU	1w	55	54	18,21,22	1.40	1 (5%)	22,30,33	1.91	5 (22%)
1	2MU	2A	2552	56,1	19,22,24	1.24	3 (15%)	26,31,36	1.92	6 (23%)
54	5MU	2y	54	54	19,22,23	1.37	6 (31%)	28,32,35	2.00	7 (25%)
54	PSU	2w	55	54	18,21,22	1.38	1 (5%)	22,30,33	1.88	4 (18%)
1	PSU	2A	1917	1	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
54	6MZ	2y	37	54,32	18,25,26	0.98	1 (5%)	16,36,39	2.00	4 (25%)
54	4SU	2w	8	54	18,21,22	1.63	4 (22%)	26,30,33	2.05	5 (19%)
32	PSU	1a	516	32	18,21,22	1.34	3 (16%)	22,30,33	1.83	4 (18%)
1	PSU	1A	1911	1	18,21,22	1.39	2 (11%)	22,30,33	1.77	3 (13%)
54	7MG	2y	46	54	22,26,27	1.35	3 (13%)	29,39,42	2.78	7 (24%)
1	2MA	1A	2503	56,1	17,25,26	0.97	0	17,37,40	1.08	2 (11%)
55	5MC	1x	32	55	18,22,23	1.01	2 (11%)	26,32,35	1.23	3 (11%)
55	PSU	1x	55	55	18,21,22	1.32	2 (11%)	22,30,33	1.97	4 (18%)
32	5MC	1a	1404	32	18,22,23	1.00	2 (11%)	26,32,35	1.19	3 (11%)
32	5MC	2a	967	32	18,22,23	0.99	2 (11%)	26,32,35	1.09	2 (7%)
32	PSU	2a	516	56,32	18,21,22	1.33	2 (11%)	22,30,33	1.83	4 (18%)
55	4SU	1x	8	55	18,21,22	2.02	4 (22%)	26,30,33	1.49	4 (15%)
55	5MU	2x	54	55	19,22,23	1.38	5 (26%)	28,32,35	2.11	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
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	1A	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	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
54	6MZ	1w	37	54	-	0/5/27/28	0/3/3/3
1	4OC	1A	1920	1	-	1/9/27/30	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	2605	56,1	-	0/7/25/26	0/2/2/2
55	5MC	2x	32	55	-	1/7/25/26	0/2/2/2
54	4SU	1y	8	54	-	2/7/25/26	0/2/2/2
1	OMG	2A	2251	56,1,55	-	0/5/27/28	0/3/3/3
43	0TD	2l	92	43	-	1/7/12/14	-
1	5MU	1A	1915	1	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	56,32	-	2/9/29/30	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
54	7MG	2w	46	54	-	2/7/37/38	0/3/3/3
54	CM0	1w	34	54	-	2/12/30/31	0/2/2/2
54	5MU	1y	54	54	-	2/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	3/7/29/30	0/3/3/3
54	CM0	2w	34	54	-	5/12/30/31	0/2/2/2
32	2MG	2a	1207	56,32	-	2/5/27/28	0/3/3/3
1	2MA	2A	2503	1	-	1/3/25/26	0/3/3/3
32	7MG	2a	527	56,32	-	3/7/37/38	0/3/3/3
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
54	7MG	1w	46	54	-	2/7/37/38	0/3/3/3
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
55	5MU	1x	54	56,55	-	0/7/25/26	0/2/2/2
32	7MG	1a	527	56,32	-	3/7/37/38	0/3/3/3
54	4SU	2y	8	54	-	2/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	3/7/12/14	-
32	5MC	2a	1404	32	-	2/7/25/26	0/2/2/2
54	7MG	1y	46	54	-	4/7/37/38	0/3/3/3
54	CM0	1y	34	54	-	2/12/30/31	0/2/2/2
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
1	OMG	1A	2251	56,1,55	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	5MC	2a	1400	32	-	4/7/25/26	0/2/2/2
1	5MU	1A	1939	1	-	0/7/25/26	0/2/2/2
55	4SU	2x	8	55	-	0/7/25/26	0/2/2/2
54	6MZ	2w	37	54	-	0/5/27/28	0/3/3/3
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	0/5/27/28	0/3/3/3
54	PSU	1y	55	54	-	0/7/25/26	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
1	4OC	2A	1920	1	-	1/9/27/30	0/2/2/2
1	5MC	2A	1962	56,1	-	2/7/25/26	0/2/2/2
1	2MU	1A	2552	56,1	-	0/9/27/28	0/2/2/2
32	MA6	1a	1518	32	-	1/7/29/30	0/3/3/3
32	5MC	2a	1407	56,32	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
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
32	4OC	2a	1402	56,32	-	2/9/29/30	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
54	PSU	2y	55	54	-	2/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	3/7/29/30	0/3/3/3
54	6MZ	1y	37	54	-	0/5/27/28	0/3/3/3
54	CM0	2y	34	53,54	-	3/12/30/31	0/2/2/2
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
1	2MU	2A	2552	56,1	-	1/9/27/28	0/2/2/2
54	5MU	2y	54	54	-	0/7/25/26	0/2/2/2
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
54	6MZ	2y	37	54,32	-	3/5/27/28	0/3/3/3
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	32	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
54	7MG	2y	46	54	-	2/7/37/38	0/3/3/3
1	2MA	1A	2503	56,1	-	2/3/25/26	0/3/3/3
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	56,32	-	0/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2

All (195) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-12.56	1.69	1.82
43	2l	92	0TD	CB-SB	-12.41	1.69	1.82
54	1y	34	CM0	C6-C5	5.63	1.40	1.34
54	2y	34	CM0	C6-C5	5.20	1.40	1.34
32	2a	966	M2G	C2-N3	5.04	1.36	1.30
54	2w	34	CM0	C6-C5	4.98	1.40	1.34
54	1w	34	CM0	C6-C5	4.95	1.39	1.34
55	2x	8	4SU	C4-N3	-4.50	1.32	1.37
54	1w	55	PSU	C6-C5	4.47	1.40	1.35
55	1x	8	4SU	C4-N3	-4.46	1.32	1.37
32	1a	966	M2G	C2-N3	4.41	1.36	1.30
54	1w	8	4SU	C4-S4	-4.34	1.60	1.68
54	2y	8	4SU	C4-S4	-4.31	1.60	1.68
54	2w	55	PSU	C6-C5	4.30	1.40	1.35
55	1x	8	4SU	C4-S4	-4.26	1.60	1.68
54	1y	8	4SU	C4-S4	-4.21	1.60	1.68
54	2w	8	4SU	C4-S4	-4.19	1.60	1.68
55	2x	8	4SU	C4-S4	-4.07	1.60	1.68
55	1x	8	4SU	C2-N3	-3.85	1.31	1.38
32	2a	527	7MG	C4-N9	-3.79	1.33	1.37
32	1a	527	7MG	C4-N9	-3.64	1.33	1.37
54	1y	55	PSU	C6-C5	3.55	1.39	1.35
55	2x	8	4SU	C2-N3	-3.51	1.31	1.38
55	2x	55	PSU	C6-C5	3.45	1.39	1.35
54	2y	55	PSU	C6-C5	3.43	1.39	1.35
54	1w	46	7MG	C4-N9	-3.40	1.33	1.37
1	2A	1911	PSU	C6-C5	3.35	1.39	1.35
32	2a	516	PSU	C6-C5	3.32	1.39	1.35
1	1A	1911	PSU	C6-C5	3.30	1.39	1.35
54	1y	8	4SU	C4-N3	-3.28	1.34	1.37
54	1y	46	7MG	C5-C4	3.26	1.48	1.38
1	2A	1917	PSU	C6-C5	3.25	1.39	1.35
54	1w	54	5MU	C6-C5	3.22	1.39	1.34
1	1A	1917	PSU	C6-C5	3.20	1.39	1.35
54	2w	46	7MG	C5-C4	3.17	1.48	1.38
55	1x	55	PSU	C6-C5	3.17	1.39	1.35
55	1x	8	4SU	C5-C4	-3.16	1.38	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1y	34	CM0	C2-N1	3.16	1.43	1.38
54	2y	46	7MG	C5-C4	3.16	1.48	1.38
1	2A	2605	PSU	C6-C5	3.13	1.39	1.35
55	1x	32	5MC	C6-C5	3.11	1.39	1.34
1	1A	2552	2MU	C4-N3	-3.09	1.33	1.38
1	1A	2251	OMG	C6-N1	-3.09	1.33	1.37
54	1y	54	5MU	C6-C5	3.03	1.39	1.34
54	1w	46	7MG	C5-C4	3.01	1.47	1.38
32	1a	516	PSU	C6-C5	3.01	1.38	1.35
54	1w	8	4SU	C4-N3	-2.98	1.34	1.37
54	2y	34	CM0	C2-N1	2.97	1.43	1.38
1	2A	2251	OMG	C6-N1	-2.97	1.33	1.37
54	2w	54	5MU	C6-C5	2.94	1.39	1.34
32	2a	1404	5MC	C6-C5	2.93	1.39	1.34
32	1a	966	M2G	C2-N2	2.90	1.40	1.35
54	2y	8	4SU	C5-C4	-2.89	1.38	1.42
1	2A	1915	5MU	C4-N3	-2.88	1.33	1.38
55	2x	8	4SU	C5-C4	-2.87	1.38	1.42
32	2a	527	7MG	C5-C4	2.85	1.47	1.38
32	1a	527	7MG	C5-C4	2.85	1.47	1.38
1	2A	1942	5MC	C6-C5	2.84	1.39	1.34
54	1y	46	7MG	C8-N9	2.83	1.47	1.46
32	2a	1407	5MC	C6-C5	2.82	1.39	1.34
1	1A	2605	PSU	C4-N3	-2.81	1.33	1.38
32	2a	967	5MC	C6-C5	2.81	1.39	1.34
55	2x	32	5MC	C6-C5	2.80	1.39	1.34
1	2A	1915	5MU	C6-C5	2.78	1.39	1.34
1	2A	1917	PSU	C4-N3	-2.78	1.33	1.38
1	2A	1939	5MU	C4-N3	-2.78	1.33	1.38
55	1x	54	5MU	C6-C5	2.75	1.39	1.34
54	2y	37	6MZ	C5-C4	2.74	1.48	1.40
32	2a	1518	MA6	C5-C4	2.74	1.48	1.40
1	2A	1939	5MU	C6-N1	-2.73	1.33	1.38
32	2a	966	M2G	C2-N2	2.73	1.40	1.35
32	1a	1207	2MG	C6-N1	-2.73	1.33	1.37
54	2w	34	CM0	C4-N3	-2.73	1.33	1.38
54	1y	37	6MZ	C5-C4	2.73	1.48	1.40
1	2A	1911	PSU	C4-N3	-2.73	1.33	1.38
1	2A	2605	PSU	C4-N3	-2.69	1.33	1.38
55	2x	54	5MU	C6-C5	2.69	1.39	1.34
1	1A	1915	5MU	C4-N3	-2.69	1.33	1.38
54	1y	34	CM0	C4-N3	-2.68	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	34	CM0	C4-N3	-2.68	1.33	1.38
1	2A	1962	5MC	C6-C5	2.67	1.39	1.34
55	1x	55	PSU	C4-N3	-2.67	1.33	1.38
1	1A	1915	5MU	C6-C5	2.67	1.39	1.34
54	2y	8	4SU	C2-N1	2.66	1.42	1.38
1	2A	2552	2MU	C4-N3	-2.66	1.33	1.38
32	2a	1519	MA6	C5-C4	2.65	1.47	1.40
1	2A	2503	2MA	C2-N3	2.65	1.36	1.31
1	1A	1939	5MU	C4-N3	-2.63	1.34	1.38
54	2w	8	4SU	C4-N3	-2.62	1.34	1.37
54	2w	46	7MG	C4-N9	-2.62	1.34	1.37
32	1a	516	PSU	C4-N3	-2.62	1.34	1.38
32	2a	1400	5MC	C6-C5	2.62	1.38	1.34
1	1A	1911	PSU	C4-N3	-2.61	1.34	1.38
55	1x	54	5MU	C4-N3	-2.60	1.34	1.38
32	1a	967	5MC	C6-C5	2.60	1.38	1.34
32	1a	1404	5MC	C6-C5	2.59	1.38	1.34
32	1a	1400	5MC	C6-C5	2.59	1.38	1.34
54	1y	8	4SU	C2-N1	2.58	1.42	1.38
1	1A	1939	5MU	C6-N1	-2.58	1.33	1.38
1	1A	1917	PSU	C4-N3	-2.57	1.34	1.38
32	1a	1404	5MC	C6-N1	-2.56	1.33	1.38
54	1y	54	5MU	C4-C5	2.56	1.49	1.44
1	1A	1939	5MU	C6-C5	2.55	1.38	1.34
54	1w	54	5MU	C4-C5	2.54	1.49	1.44
54	2w	54	5MU	C4-N3	-2.53	1.34	1.38
55	2x	54	5MU	C4-N3	-2.53	1.34	1.38
54	2y	54	5MU	C6-C5	2.53	1.38	1.34
1	2A	1915	5MU	C2-N1	2.51	1.42	1.38
32	1a	1518	MA6	C5-C4	2.51	1.47	1.40
54	2w	37	6MZ	C5-C4	2.51	1.47	1.40
32	1a	1498	UR3	C2-N1	2.50	1.42	1.38
1	1A	2605	PSU	C2-N1	-2.50	1.33	1.36
32	1a	966	M2G	C6-N1	-2.48	1.34	1.37
32	1a	1407	5MC	C6-C5	2.47	1.38	1.34
32	1a	1519	MA6	C5-C4	2.47	1.47	1.40
54	2y	55	PSU	C4-N3	-2.47	1.34	1.38
32	2a	527	7MG	C6-N1	-2.46	1.34	1.38
1	1A	1915	5MU	C4-C5	2.46	1.48	1.44
55	2x	55	PSU	C4-N3	-2.46	1.34	1.38
55	2x	54	5MU	C4-C5	2.46	1.48	1.44
54	2y	54	5MU	C4-C5	2.46	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1y	46	7MG	C6-N1	-2.45	1.34	1.38
54	1w	37	6MZ	C5-C4	2.45	1.47	1.40
32	2a	516	PSU	C4-N3	-2.45	1.34	1.38
1	2A	1939	5MU	C4-C5	2.45	1.48	1.44
1	1A	1942	5MC	C6-N1	-2.45	1.33	1.38
1	1A	1962	5MC	C6-C5	2.44	1.38	1.34
54	2y	8	4SU	C4-N3	-2.44	1.35	1.37
54	2y	46	7MG	C8-N9	2.43	1.47	1.46
54	1y	54	5MU	C4-N3	-2.42	1.34	1.38
54	1y	55	PSU	C4-N3	-2.41	1.34	1.38
54	2y	46	7MG	C6-N1	-2.41	1.34	1.38
1	2A	1962	5MC	C6-N1	-2.40	1.33	1.38
1	2A	1939	5MU	C6-C5	2.39	1.38	1.34
1	1A	1942	5MC	C6-C5	2.39	1.38	1.34
1	2A	1939	5MU	C2-N3	-2.38	1.33	1.38
54	1w	8	4SU	C5-C4	-2.37	1.39	1.42
1	2A	1915	5MU	C4-C5	2.36	1.48	1.44
1	1A	1915	5MU	C2-N1	2.36	1.42	1.38
54	2y	54	5MU	C4-N3	-2.36	1.34	1.38
32	2a	966	M2G	C6-N1	-2.35	1.34	1.37
55	1x	54	5MU	C2-N1	2.34	1.42	1.38
54	2w	8	4SU	C2-N1	2.34	1.42	1.38
32	2a	1207	2MG	C6-N1	-2.34	1.34	1.37
1	1A	2552	2MU	C2-N3	-2.33	1.33	1.38
1	1A	2605	PSU	C2-N3	-2.32	1.33	1.37
32	1a	967	5MC	C6-N1	-2.32	1.34	1.38
1	2A	1915	5MU	C6-N1	-2.31	1.34	1.38
54	2w	46	7MG	C8-N9	2.30	1.47	1.46
1	1A	1962	5MC	C6-N1	-2.29	1.34	1.38
55	1x	54	5MU	C4-C5	2.27	1.48	1.44
32	1a	1400	5MC	C6-N1	-2.26	1.34	1.38
54	2w	8	4SU	C5-C4	-2.25	1.39	1.42
32	1a	1407	5MC	C6-N1	-2.24	1.34	1.38
32	2a	1400	5MC	C6-N1	-2.23	1.34	1.38
54	2y	54	5MU	C2-N1	2.23	1.42	1.38
54	1y	8	4SU	C5-C4	-2.22	1.39	1.42
1	2A	2552	2MU	C5-C4	2.22	1.48	1.43
32	2a	967	5MC	C6-N1	-2.21	1.34	1.38
55	1x	32	5MC	C6-N1	-2.20	1.34	1.38
1	2A	1942	5MC	C6-N1	-2.19	1.34	1.38
54	2w	54	5MU	C2-N1	2.19	1.42	1.38
54	1y	54	5MU	C2-N1	2.18	1.41	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1939	5MU	C4-C5	2.18	1.48	1.44
54	1w	8	4SU	C2-N3	-2.17	1.34	1.38
54	2w	34	CM0	C2-N1	2.17	1.41	1.38
54	1w	54	5MU	C4-N3	-2.15	1.34	1.38
1	1A	1915	5MU	C6-N1	-2.14	1.34	1.38
1	1A	1939	5MU	C2-N3	-2.14	1.34	1.38
54	2y	54	5MU	C6-N1	-2.14	1.34	1.38
54	1w	54	5MU	C6-N1	-2.13	1.34	1.38
32	2a	1498	UR3	C2-N1	2.13	1.41	1.38
54	1w	34	CM0	C2-N3	-2.13	1.34	1.38
54	1w	46	7MG	C6-N1	-2.13	1.34	1.38
32	1a	516	PSU	C2-N3	-2.13	1.33	1.37
54	2w	54	5MU	C4-C5	2.12	1.48	1.44
1	2A	2605	PSU	C2-N3	-2.11	1.33	1.37
54	1y	54	5MU	C6-N1	-2.10	1.34	1.38
55	2x	54	5MU	C6-N1	-2.10	1.34	1.38
55	1x	54	5MU	C6-N1	-2.09	1.34	1.38
32	2a	1404	5MC	C6-N1	-2.09	1.34	1.38
54	2w	46	7MG	C6-N1	-2.09	1.35	1.38
55	2x	54	5MU	C2-N1	2.08	1.41	1.38
55	2x	32	5MC	C6-N1	-2.08	1.34	1.38
54	2y	54	5MU	C2-N3	-2.07	1.34	1.38
32	2a	1407	5MC	C6-N1	-2.07	1.34	1.38
54	1y	8	4SU	C6-C5	2.06	1.39	1.35
1	2A	2552	2MU	C2-N3	-2.06	1.34	1.38
54	1w	54	5MU	C2-N1	2.06	1.41	1.38
54	1y	37	6MZ	C2-N3	2.05	1.35	1.32
32	1a	527	7MG	C6-N1	-2.05	1.35	1.38
54	1w	8	4SU	C2-N1	2.02	1.41	1.38
32	2a	527	7MG	C5-C6	2.02	1.48	1.43
32	1a	527	7MG	C8-N9	2.01	1.47	1.46
54	1w	54	5MU	C2-N3	-2.01	1.34	1.38

All (309) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	2y	46	7MG	N9-C4-N3	10.26	140.81	125.47
54	1y	46	7MG	N9-C4-N3	9.65	139.90	125.47
43	1l	92	0TD	CSB-SB-CB	9.09	118.88	102.44
54	2w	46	7MG	N9-C4-N3	8.97	138.89	125.47
54	1w	46	7MG	N9-C4-N3	8.53	138.23	125.47
32	1a	527	7MG	N9-C4-N3	8.09	137.57	125.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	527	7MG	N9-C4-N3	8.00	137.43	125.47
54	2y	34	CM0	C4-N3-C2	-6.38	119.10	127.35
54	2w	8	4SU	C4-N3-C2	-6.26	121.26	127.34
54	2y	46	7MG	C5-C4-N3	-6.23	116.26	128.13
54	1y	55	PSU	N1-C2-N3	6.20	122.16	115.13
55	1x	55	PSU	N1-C2-N3	6.10	122.04	115.13
54	1y	37	6MZ	C2-N1-C6	6.07	121.80	116.59
1	1A	2605	PSU	N1-C2-N3	5.96	121.88	115.13
1	2A	1917	PSU	N1-C2-N3	5.96	121.88	115.13
1	1A	1917	PSU	N1-C2-N3	5.92	121.84	115.13
1	2A	1939	5MU	C4-N3-C2	-5.90	119.71	127.35
1	2A	2605	PSU	N1-C2-N3	5.88	121.80	115.13
32	2a	1498	UR3	C4-N3-C2	-5.88	119.03	124.56
54	2y	55	PSU	N1-C2-N3	5.87	121.78	115.13
54	1w	8	4SU	C5-C4-N3	5.84	120.10	114.69
54	1w	37	6MZ	C2-N1-C6	5.83	121.59	116.59
54	1w	54	5MU	C4-N3-C2	-5.82	119.82	127.35
54	1w	8	4SU	C4-N3-C2	-5.76	121.75	127.34
1	2A	1911	PSU	N1-C2-N3	5.76	121.65	115.13
54	2y	37	6MZ	C2-N1-C6	5.71	121.49	116.59
32	2a	516	PSU	N1-C2-N3	5.67	121.56	115.13
55	2x	55	PSU	N1-C2-N3	5.65	121.53	115.13
54	1y	34	CM0	C7-O5-C5	5.65	124.97	117.58
32	1a	1498	UR3	C4-N3-C2	-5.65	119.25	124.56
54	1w	46	7MG	N9-C8-N7	-5.64	95.31	103.38
32	1a	516	PSU	N1-C2-N3	5.64	121.52	115.13
1	1A	2552	2MU	N3-C2-N1	5.56	122.27	114.89
32	2a	527	7MG	N9-C8-N7	-5.55	95.44	103.38
54	2w	8	4SU	C5-C4-N3	5.53	119.82	114.69
54	2w	55	PSU	N1-C2-N3	5.52	121.39	115.13
54	2y	8	4SU	C5-C4-N3	5.49	119.78	114.69
1	2A	1915	5MU	C4-N3-C2	-5.48	120.26	127.35
54	2w	37	6MZ	C2-N1-C6	5.48	121.29	116.59
1	1A	1911	PSU	N1-C2-N3	5.48	121.33	115.13
54	1y	34	CM0	N3-C2-N1	5.45	122.13	114.89
54	1w	55	PSU	N1-C2-N3	5.45	121.31	115.13
1	1A	1939	5MU	C4-N3-C2	-5.45	120.30	127.35
54	1y	8	4SU	C4-N3-C2	-5.36	122.14	127.34
54	2w	46	7MG	C5-C4-N3	-5.34	117.95	128.13
32	1a	527	7MG	N9-C8-N7	-5.32	95.77	103.38
54	1y	46	7MG	C5-C4-N3	-5.29	118.06	128.13
54	2y	34	CM0	N3-C2-N1	5.28	121.90	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	2x	54	5MU	C4-N3-C2	-5.28	120.52	127.35
1	1A	1915	5MU	C4-N3-C2	-5.26	120.54	127.35
54	1w	54	5MU	N3-C2-N1	5.25	121.86	114.89
54	2w	34	CM0	C4-N3-C2	-5.21	120.61	127.35
55	2x	54	5MU	N3-C2-N1	5.21	121.80	114.89
1	2A	1939	5MU	N3-C2-N1	5.18	121.77	114.89
54	1w	34	CM0	N3-C2-N1	5.16	121.74	114.89
54	1y	54	5MU	N3-C2-N1	5.16	121.74	114.89
54	2y	8	4SU	C4-N3-C2	-5.16	122.33	127.34
54	1y	54	5MU	C4-N3-C2	-5.12	120.72	127.35
54	2w	46	7MG	N9-C8-N7	-5.08	96.11	103.38
43	2l	92	0TD	CSB-SB-CB	-5.08	93.25	102.44
1	2A	2552	2MU	N3-C2-N1	5.06	121.61	114.89
32	1a	527	7MG	C5-C4-N3	-5.04	118.53	128.13
1	1A	1915	5MU	N3-C2-N1	5.01	121.54	114.89
54	1y	8	4SU	C5-C4-N3	5.01	119.33	114.69
54	2y	8	4SU	C1'-N1-C2	4.99	126.61	117.57
54	2w	34	CM0	N3-C2-N1	4.97	121.49	114.89
54	1w	34	CM0	C4-N3-C2	-4.96	120.93	127.35
54	1w	46	7MG	C5-C4-N3	-4.95	118.69	128.13
1	2A	1915	5MU	C5-C4-N3	4.94	119.53	115.31
54	1y	34	CM0	C4-N3-C2	-4.93	120.96	127.35
1	2A	1939	5MU	C5-C4-N3	4.92	119.51	115.31
1	2A	1915	5MU	N3-C2-N1	4.92	121.42	114.89
32	2a	527	7MG	C5-C4-N3	-4.91	118.77	128.13
54	2y	46	7MG	C2-N3-C4	4.90	121.04	112.30
1	1A	1939	5MU	C5-C4-N3	4.90	119.49	115.31
55	1x	54	5MU	N3-C2-N1	4.86	121.34	114.89
54	2y	54	5MU	C4-N3-C2	-4.84	121.09	127.35
54	1y	46	7MG	N9-C8-N7	-4.83	96.47	103.38
54	1w	54	5MU	C5-C4-N3	4.82	119.42	115.31
1	1A	1915	5MU	C5-C4-N3	4.75	119.36	115.31
54	1w	54	5MU	C5-C6-N1	-4.75	118.45	123.34
1	1A	1939	5MU	O4-C4-C5	-4.70	119.45	124.90
55	1x	54	5MU	C4-N3-C2	-4.70	121.27	127.35
54	2y	8	4SU	C5-C4-S4	-4.70	118.42	124.47
1	2A	1939	5MU	C5-C6-N1	-4.68	118.52	123.34
1	2A	2552	2MU	C4-N3-C2	-4.67	120.42	126.58
54	1w	54	5MU	O4-C4-C5	-4.63	119.54	124.90
54	2w	54	5MU	C4-N3-C2	-4.59	121.41	127.35
1	1A	1939	5MU	N3-C2-N1	4.55	120.94	114.89
54	2y	46	7MG	N9-C8-N7	-4.55	96.87	103.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	2y	54	5MU	N3-C2-N1	4.54	120.92	114.89
1	1A	1939	5MU	C5-C6-N1	-4.52	118.69	123.34
54	2w	54	5MU	N3-C2-N1	4.51	120.87	114.89
54	1y	54	5MU	C5-C4-N3	4.37	119.04	115.31
54	1y	46	7MG	C2-N3-C4	4.36	120.07	112.30
32	1a	527	7MG	C2-N3-C4	4.36	120.06	112.30
55	2x	54	5MU	C5-C4-N3	4.34	119.02	115.31
54	2y	54	5MU	C5-C4-N3	4.32	119.00	115.31
1	2A	1915	5MU	C5-C6-N1	-4.23	118.98	123.34
54	2w	46	7MG	C2-N3-C4	4.23	119.83	112.30
55	1x	55	PSU	C4-N3-C2	-4.22	120.26	126.34
1	2A	2605	PSU	C4-N3-C2	-4.19	120.30	126.34
1	1A	2605	PSU	C4-N3-C2	-4.18	120.31	126.34
1	1A	2552	2MU	C4-N3-C2	-4.18	121.06	126.58
55	1x	32	5MC	C5-C6-N1	-4.11	119.11	123.34
54	1w	37	6MZ	C9-N6-C6	-4.07	119.37	122.87
32	2a	527	7MG	C2-N3-C4	4.06	119.54	112.30
54	2w	37	6MZ	C9-N6-C6	-4.05	119.38	122.87
1	1A	1962	5MC	C5-C6-N1	-4.05	119.17	123.34
55	2x	55	PSU	C4-N3-C2	-4.02	120.55	126.34
54	1w	46	7MG	C2-N3-C4	4.02	119.46	112.30
55	1x	8	4SU	C5-C4-N3	4.01	118.41	114.69
54	1y	55	PSU	O2-C2-N1	-3.97	118.42	122.79
55	1x	8	4SU	C6-C5-C4	-3.95	116.53	119.95
54	2y	34	CM0	C7-O5-C5	3.94	122.74	117.58
1	1A	2552	2MU	O2-C2-N1	-3.93	117.56	122.79
32	1a	516	PSU	C4-N3-C2	-3.92	120.69	126.34
54	2w	54	5MU	O4-C4-C5	-3.92	120.36	124.90
32	2a	516	PSU	C4-N3-C2	-3.91	120.71	126.34
55	2x	32	5MC	C5-C6-N1	-3.91	119.32	123.34
1	2A	1939	5MU	O4-C4-C5	-3.90	120.39	124.90
54	1y	54	5MU	O4-C4-C5	-3.89	120.39	124.90
1	1A	1917	PSU	C4-N3-C2	-3.89	120.73	126.34
1	1A	1915	5MU	O4-C4-C5	-3.89	120.39	124.90
54	2w	54	5MU	C5-C4-N3	3.87	118.62	115.31
55	2x	54	5MU	O4-C4-C5	-3.85	120.44	124.90
55	1x	54	5MU	C5-C4-N3	3.85	118.59	115.31
54	2w	55	PSU	O2-C2-N1	-3.83	118.57	122.79
54	2y	54	5MU	O4-C4-C5	-3.83	120.47	124.90
32	1a	1400	5MC	C5-C6-N1	-3.81	119.42	123.34
54	1y	55	PSU	C4-N3-C2	-3.79	120.88	126.34
1	1A	2552	2MU	C2'-C1'-N1	-3.78	106.88	114.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	1518	MA6	C4-C5-N7	-3.78	105.46	109.40
54	1y	8	4SU	N3-C2-N1	3.77	119.89	114.89
1	2A	1917	PSU	C4-N3-C2	-3.71	120.99	126.34
1	2A	1911	PSU	C4-N3-C2	-3.70	121.01	126.34
55	1x	54	5MU	O4-C4-C5	-3.69	120.62	124.90
54	1w	55	PSU	C4-N3-C2	-3.69	121.02	126.34
54	2w	8	4SU	N3-C2-N1	3.69	119.79	114.89
1	2A	1915	5MU	O4-C4-C5	-3.69	120.63	124.90
32	2a	1407	5MC	C5-C6-N1	-3.65	119.58	123.34
54	2y	55	PSU	C4-N3-C2	-3.63	121.10	126.34
32	1a	1519	MA6	C9-N6-C6	-3.60	108.63	119.51
54	1w	55	PSU	O2-C2-N1	-3.58	118.84	122.79
54	2w	54	5MU	C5-C6-N1	-3.56	119.67	123.34
54	1y	37	6MZ	C9-N6-C6	-3.55	119.82	122.87
32	2a	1400	5MC	C5-C6-N1	-3.54	119.69	123.34
1	2A	2552	2MU	O2-C2-N1	-3.54	118.08	122.79
54	2w	55	PSU	C4-N3-C2	-3.53	121.25	126.34
32	2a	967	5MC	C5-C6-N1	-3.51	119.72	123.34
32	2a	1518	MA6	C9-N6-C6	-3.50	108.91	119.51
54	2w	8	4SU	C5-C4-S4	-3.50	119.96	124.47
1	1A	1911	PSU	C4-N3-C2	-3.49	121.31	126.34
1	1A	2605	PSU	O2-C2-N1	-3.48	118.96	122.79
54	1w	54	5MU	O2-C2-N1	-3.45	118.21	122.79
55	2x	54	5MU	C5-C6-N1	-3.45	119.79	123.34
1	1A	1942	5MC	C5-C6-N1	-3.44	119.80	123.34
55	2x	8	4SU	C5-C4-N3	3.42	117.86	114.69
1	2A	1917	PSU	O2-C2-N1	-3.42	119.03	122.79
54	1y	8	4SU	C1'-N1-C2	3.41	123.75	117.57
55	1x	55	PSU	O2-C2-N1	-3.39	119.05	122.79
54	2y	37	6MZ	C9-N6-C6	-3.39	119.95	122.87
1	1A	1915	5MU	C5-C6-N1	-3.36	119.88	123.34
32	2a	1519	MA6	C4-C5-N7	-3.35	105.90	109.40
54	1y	46	7MG	C5-C4-N9	-3.32	102.04	106.35
54	2y	55	PSU	O2-C2-N1	-3.32	119.14	122.79
32	2a	1404	5MC	C5-C6-N1	-3.31	119.93	123.34
1	2A	1942	5MC	C5-C6-N1	-3.29	119.95	123.34
54	2y	54	5MU	C5-C6-N1	-3.27	119.97	123.34
1	1A	1917	PSU	O2-C2-N1	-3.27	119.19	122.79
54	1w	8	4SU	N3-C2-N1	3.26	119.22	114.89
54	1y	37	6MZ	N3-C2-N1	-3.26	123.59	128.68
43	1l	92	0TD	OD2-CG-CB	3.25	120.17	113.15
54	1y	37	6MZ	C4-C5-N7	-3.24	106.02	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	1a	1519	MA6	N3-C2-N1	-3.23	123.63	128.68
32	2a	1519	MA6	N3-C2-N1	-3.21	123.66	128.68
1	2A	1911	PSU	O2-C2-N1	-3.21	119.26	122.79
32	1a	967	5MC	C5-C6-N1	-3.21	120.04	123.34
43	2l	92	0TD	OD2-CG-CB	3.20	120.07	113.15
32	2a	1519	MA6	C9-N6-C6	-3.20	109.82	119.51
54	1y	54	5MU	C5-C6-N1	-3.19	120.06	123.34
32	1a	1404	5MC	C5-C6-N1	-3.19	120.06	123.34
32	1a	1518	MA6	C4-C5-N7	-3.18	106.08	109.40
55	1x	54	5MU	C5-C6-N1	-3.18	120.06	123.34
1	1A	1911	PSU	O2-C2-N1	-3.17	119.30	122.79
54	1w	8	4SU	C5-C4-S4	-3.17	120.39	124.47
55	2x	32	5MC	O2-C2-N3	-3.14	117.22	122.33
32	1a	1518	MA6	N3-C2-N1	-3.14	123.77	128.68
54	2y	8	4SU	C1'-N1-C6	-3.12	114.04	120.84
55	2x	8	4SU	C6-C5-C4	-3.11	117.25	119.95
1	2A	1962	5MC	C5-C6-N1	-3.09	120.16	123.34
32	2a	1518	MA6	N3-C2-N1	-3.09	123.85	128.68
54	1w	37	6MZ	N3-C2-N1	-3.06	123.89	128.68
55	2x	54	5MU	O2-C2-N1	-3.06	118.72	122.79
54	2w	54	5MU	O2-C2-N1	-3.03	118.75	122.79
1	2A	2605	PSU	O2-C2-N1	-3.02	119.47	122.79
54	2y	37	6MZ	C4-C5-N7	-3.00	106.28	109.40
1	2A	2552	2MU	C2'-C1'-N1	-2.93	108.53	114.22
1	2A	2552	2MU	C5-C4-N3	2.93	119.22	114.84
32	1a	1518	MA6	N1-C6-N6	2.90	120.11	117.06
1	1A	1939	5MU	O2-C2-N1	-2.88	118.96	122.79
54	1w	37	6MZ	C4-C5-N7	-2.86	106.42	109.40
55	1x	8	4SU	O2-C2-N1	2.85	126.58	122.79
54	2w	37	6MZ	N3-C2-N1	-2.84	124.25	128.68
54	2y	46	7MG	C5-C6-N1	2.82	115.96	110.99
1	2A	1962	5MC	C5-C4-N3	-2.81	118.64	121.67
32	1a	1519	MA6	N1-C6-N6	2.81	120.01	117.06
32	2a	516	PSU	O2-C2-N1	-2.80	119.71	122.79
32	1a	1407	5MC	C5-C6-N1	-2.79	120.47	123.34
54	2w	37	6MZ	C4-C5-N7	-2.78	106.50	109.40
55	1x	32	5MC	C5-C4-N3	-2.76	118.69	121.67
1	2A	1939	5MU	O2-C2-N1	-2.76	119.12	122.79
32	1a	1519	MA6	C4-C5-N7	-2.75	106.54	109.40
54	2y	8	4SU	N3-C2-N1	2.74	118.53	114.89
32	1a	527	7MG	C5-C6-N1	2.74	115.82	110.99
1	2A	2552	2MU	O4-C4-C5	-2.73	120.36	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	1a	1402	4OC	C6-C5-C4	2.72	120.29	116.96
54	1w	34	CM0	C7-O5-C5	2.71	121.12	117.58
54	2y	34	CM0	O2-C2-N1	-2.70	119.19	122.79
55	2x	55	PSU	O2-C2-N1	-2.70	119.82	122.79
32	1a	1518	MA6	C9-N6-C6	-2.68	111.40	119.51
32	2a	1407	5MC	C5-C4-N3	-2.67	118.80	121.67
54	2w	34	CM0	C7-O5-C5	2.66	121.06	117.58
32	1a	1407	5MC	C5-C4-N3	-2.66	118.80	121.67
1	1A	2251	OMG	C5-C6-N1	2.64	118.61	113.95
54	2y	46	7MG	C5-C4-N9	-2.64	102.93	106.35
55	2x	8	4SU	C1'-N1-C2	2.63	122.33	117.57
54	2w	34	CM0	O2-C2-N1	-2.63	119.30	122.79
32	2a	1518	MA6	C10-N6-C9	-2.62	107.69	116.12
32	1a	1207	2MG	C8-N7-C5	2.62	107.97	102.99
32	2a	527	7MG	C5-C6-N1	2.62	115.60	110.99
32	1a	516	PSU	O2-C2-N1	-2.61	119.91	122.79
54	2y	37	6MZ	N3-C2-N1	-2.60	124.62	128.68
54	1y	54	5MU	O2-C2-N1	-2.58	119.36	122.79
1	2A	2251	OMG	C5-C6-N1	2.58	118.50	113.95
54	2w	46	7MG	C5-C6-N1	2.56	115.51	110.99
32	1a	1404	5MC	C5-C4-N3	-2.56	118.91	121.67
32	1a	1498	UR3	C1'-N1-C2	2.55	121.29	116.99
1	1A	2503	2MA	C8-N7-C5	2.53	107.81	102.99
1	1A	1915	5MU	O2-C2-N1	-2.53	119.43	122.79
32	2a	967	5MC	C5-C4-N3	-2.53	118.95	121.67
1	1A	1942	5MC	C5-C4-N3	-2.52	118.95	121.67
54	1w	46	7MG	C5-C4-N9	-2.52	103.08	106.35
32	1a	967	5MC	C5-C4-N3	-2.51	118.97	121.67
54	1w	55	PSU	C6-C5-C4	-2.49	116.45	118.20
1	1A	2503	2MA	C5-C6-N1	2.49	118.31	114.02
1	2A	2503	2MA	C5-C6-N1	2.49	118.31	114.02
55	2x	8	4SU	O2-C2-N1	2.49	126.09	122.79
32	2a	1404	5MC	C5-C4-N3	-2.49	118.99	121.67
54	2w	46	7MG	C5-C4-N9	-2.45	103.16	106.35
1	2A	1942	5MC	C5-C4-N3	-2.44	119.04	121.67
54	2y	54	5MU	C5M-C5-C4	2.44	121.45	118.77
54	1w	34	CM0	O2-C2-N1	-2.44	119.55	122.79
55	2x	32	5MC	C5-C4-N3	-2.41	119.08	121.67
54	2y	46	7MG	O6-C6-C5	-2.41	121.64	127.54
43	2l	92	0TD	OD1-CG-CB	-2.38	117.45	122.44
1	1A	2552	2MU	O4-C4-C5	-2.38	120.97	125.16
54	1y	8	4SU	C5-C4-S4	-2.37	121.41	124.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	1402	4OC	C6-C5-C4	2.37	119.86	116.96
54	1y	34	CM0	O2-C2-N3	-2.37	117.09	121.50
32	1a	966	M2G	C8-N7-C5	2.35	107.47	102.99
55	2x	8	4SU	O2-C2-N3	-2.34	117.13	121.50
32	2a	1402	4OC	CM4-N4-C4	-2.34	117.88	122.45
1	1A	2552	2MU	C5-C4-N3	2.34	118.34	114.84
32	1a	966	M2G	C5-C6-N1	2.33	118.07	113.95
54	1w	46	7MG	C5-C6-N1	2.33	115.10	110.99
32	1a	527	7MG	O6-C6-C5	-2.32	121.84	127.54
32	2a	1207	2MG	C8-N7-C5	2.30	107.38	102.99
1	1A	2251	OMG	C8-N7-C5	2.30	107.37	102.99
32	2a	1404	5MC	O2-C2-N3	-2.30	118.59	122.33
54	1y	46	7MG	C5-C6-N1	2.30	115.04	110.99
1	2A	2605	PSU	C5-C6-N1	-2.28	118.69	122.11
32	1a	1498	UR3	C3U-N3-C2	2.25	121.26	117.31
32	1a	1518	MA6	C10-N6-C9	-2.23	108.92	116.12
32	1a	1404	5MC	O2-C2-N3	-2.20	118.75	122.33
32	1a	1400	5MC	C5-C4-N3	-2.20	119.30	121.67
32	2a	966	M2G	C5-C6-N1	2.20	117.83	113.95
55	2x	55	PSU	C5-C6-N1	-2.20	118.82	122.11
54	2w	8	4SU	C1'-N1-C2	2.19	121.54	117.57
1	2A	1920	4OC	O2-C2-N3	-2.19	118.77	122.33
1	2A	1915	5MU	O2-C2-N1	-2.18	119.89	122.79
55	1x	55	PSU	C5-C6-N1	-2.18	118.84	122.11
43	1l	92	0TD	OD1-CG-CB	-2.18	117.88	122.44
1	2A	2251	OMG	C8-N7-C5	2.17	107.11	102.99
32	1a	1518	MA6	C10-N6-C6	-2.16	112.99	119.51
54	2w	55	PSU	O4-C4-C5	-2.15	118.42	124.05
1	1A	1920	4OC	CM2-O2'-C2'	-2.15	108.89	114.52
32	2a	966	M2G	C8-N7-C5	2.13	107.04	102.99
1	2A	2251	OMG	O6-C6-C5	-2.13	120.22	124.37
55	1x	32	5MC	O2-C2-N3	-2.12	118.88	122.33
54	2w	46	7MG	O6-C6-C5	-2.12	122.34	127.54
54	2y	54	5MU	O2-C2-N1	-2.12	119.97	122.79
54	1y	46	7MG	CM7-N7-C5	2.11	131.86	126.40
54	1w	55	PSU	O4-C4-C5	-2.09	118.58	124.05
32	1a	516	PSU	O4'-C1'-C2'	2.09	108.09	105.14
1	1A	2605	PSU	C5-C6-N1	-2.08	118.98	122.11
1	1A	1915	5MU	C5M-C5-C4	2.08	121.05	118.77
1	2A	2503	2MA	C8-N7-C5	2.08	106.94	102.99
32	2a	1519	MA6	N1-C6-N6	2.07	119.24	117.06
32	1a	527	7MG	CM7-N7-C5	2.07	131.74	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	1400	5MC	C5-C4-N3	-2.07	119.44	121.67
32	2a	516	PSU	O4'-C1'-C2'	2.05	108.04	105.14
55	2x	54	5MU	C5M-C5-C4	2.05	121.02	118.77
1	2A	1939	5MU	C5M-C5-C6	-2.04	120.12	122.85
55	1x	54	5MU	O2-C2-N1	-2.04	120.07	122.79
55	1x	8	4SU	C1'-N1-C2	2.04	121.26	117.57
54	1y	55	PSU	O4'-C1'-C2'	2.01	107.98	105.14
32	2a	1498	UR3	C1'-N1-C2	2.01	120.38	116.99
32	2a	527	7MG	CM7-N7-C5	2.01	131.57	126.40

There are no chirality outliers.

All (75) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
43	1l	92	0TD	O-C-CA-CB
43	1l	92	0TD	CG-CB-SB-CSB
32	2a	1207	2MG	C3'-C4'-C5'-O5'
32	2a	1518	MA6	C5-C6-N6-C9
32	2a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C5-C6-N6-C10
54	1w	46	7MG	O4'-C4'-C5'-O5'
54	1y	46	7MG	C4'-C5'-O5'-P
54	2y	46	7MG	C2'-C1'-N9-C8
54	1y	54	5MU	C3'-C4'-C5'-O5'
54	1y	54	5MU	O4'-C4'-C5'-O5'
32	1a	1402	4OC	O4'-C4'-C5'-O5'
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	527	7MG	C3'-C4'-C5'-O5'
32	2a	1207	2MG	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
54	1w	46	7MG	C3'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
54	2w	46	7MG	O4'-C4'-C5'-O5'
32	2a	1518	MA6	N1-C6-N6-C9
54	2w	34	CM0	O5-C7-C8-O8
54	2w	34	CM0	O5-C7-C8-O9
32	1a	1402	4OC	C3'-C4'-C5'-O5'
54	2w	46	7MG	C3'-C4'-C5'-O5'
54	1y	34	CM0	O5-C7-C8-O8
32	1a	527	7MG	C3'-C4'-C5'-O5'
32	2a	527	7MG	O4'-C4'-C5'-O5'
32	1a	1518	MA6	C5-C6-N6-C10

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Mol	Chain	Res	Type	Atoms
32	1a	1519	MA6	C5-C6-N6-C10
32	2a	1518	MA6	C5-C6-N6-C10
54	1y	46	7MG	C3'-C4'-C5'-O5'
54	2w	34	CM0	C6-C5-O5-C7
54	2w	34	CM0	C4-C5-O5-C7
32	2a	1402	4OC	O4'-C4'-C5'-O5'
32	2a	1400	5MC	C2'-C1'-N1-C6
43	2l	92	0TD	CG-CB-SB-CSB
32	1a	527	7MG	O4'-C4'-C5'-O5'
54	1y	34	CM0	O5-C7-C8-O9
54	2w	34	CM0	C8-C7-O5-C5
54	2y	34	CM0	C8-C7-O5-C5
54	1y	46	7MG	C2'-C1'-N9-C8
32	2a	1404	5MC	C3'-C4'-C5'-O5'
32	1a	527	7MG	C4'-C5'-O5'-P
54	2y	37	6MZ	C3'-C4'-C5'-O5'
54	2y	37	6MZ	C4'-C5'-O5'-P
1	2A	2552	2MU	O4'-C4'-C5'-O5'
32	2a	1404	5MC	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C4'-C5'-O5'-P
32	2a	1400	5MC	O4'-C1'-N1-C6
54	1w	34	CM0	O5-C7-C8-O8
54	2y	55	PSU	O4'-C1'-C5-C4
54	2y	46	7MG	C2'-C1'-N9-C4
54	1y	8	4SU	C2'-C1'-N1-C6
54	2y	8	4SU	C2'-C1'-N1-C6
54	1y	46	7MG	O4'-C1'-N9-C8
32	2a	1400	5MC	O4'-C1'-N1-C2
43	1l	92	0TD	CA-CB-SB-CSB
32	2a	1400	5MC	C2'-C1'-N1-C2
1	2A	1962	5MC	C2'-C1'-N1-C6
1	2A	1962	5MC	O4'-C1'-N1-C6
54	2y	55	PSU	O4'-C1'-C5-C6
54	1y	8	4SU	C2'-C1'-N1-C2
54	2y	8	4SU	C2'-C1'-N1-C2
1	1A	2503	2MA	C4'-C5'-O5'-P
32	2a	1402	4OC	C3'-C4'-C5'-O5'
54	2y	34	CM0	O4'-C4'-C5'-O5'
54	1w	34	CM0	O5-C7-C8-O9
1	2A	1920	4OC	C2'-C1'-N1-C2
1	1A	1920	4OC	C2'-C1'-N1-C2
55	2x	32	5MC	C2'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
54	2y	34	CM0	O5-C7-C8-O9
1	2A	2503	2MA	O4'-C4'-C5'-O5'
1	1A	2503	2MA	O4'-C4'-C5'-O5'
54	2y	37	6MZ	O4'-C4'-C5'-O5'
32	2a	527	7MG	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2801 ligands modelled in this entry, 2797 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
57	DI0	1A	4098	-	58,61,61	2.41	23 (39%)	77,92,92	2.13	25 (32%)
60	SF4	2d	303	35	0,12,12	-	-	-		
57	DI0	2A	3846	-	58,61,61	1.03	2 (3%)	77,92,92	1.57	15 (19%)
60	SF4	1d	3102	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	DI0	1A	4098	-	-	10/70/121/121	0/3/4/4
60	SF4	2d	303	35	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	DI0	2A	3846	-	-	10/70/121/121	0/3/4/4
60	SF4	1d	3102	35	-	-	0/6/5/5

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	1A	4098	DI0	CAF-CAE	-6.43	1.37	1.51
57	1A	4098	DI0	OBJ-CAP	-5.51	1.35	1.44
57	2A	3846	DI0	CAF-CAE	-5.31	1.39	1.51
57	1A	4098	DI0	OBH-CAD	-4.58	1.36	1.44
57	1A	4098	DI0	OBK-CAN	-4.29	1.35	1.44
57	1A	4098	DI0	CBC-CBB	-4.17	1.48	1.54
57	1A	4098	DI0	OAU-CBG	-4.06	1.36	1.44
57	1A	4098	DI0	OAY-CAR	-3.99	1.31	1.41
57	1A	4098	DI0	CAP-CAH	-3.84	1.47	1.55
57	1A	4098	DI0	OAL-CAW	-3.78	1.39	1.46
57	1A	4098	DI0	CBD-CBG	-3.52	1.45	1.51
57	1A	4098	DI0	OAM-CAB	-3.43	1.32	1.41
57	1A	4098	DI0	OAM-CAH	-3.29	1.35	1.44
57	1A	4098	DI0	CAZ-CAX	-2.95	1.46	1.53
57	1A	4098	DI0	CBC-CAP	-2.92	1.49	1.54
57	1A	4098	DI0	OBI-CAG	-2.80	1.36	1.43
57	1A	4098	DI0	OBL-CAX	-2.78	1.37	1.42
57	1A	4098	DI0	CAD-CAW	-2.53	1.50	1.54
57	1A	4098	DI0	CBQ-CAN	-2.50	1.46	1.52
57	1A	4098	DI0	CAD-CAA	-2.46	1.49	1.54
57	2A	3846	DI0	OAM-CAB	2.14	1.47	1.41
57	1A	4098	DI0	OAV-CAR	-2.14	1.37	1.42
57	1A	4098	DI0	OAV-CAZ	-2.13	1.39	1.44
57	1A	4098	DI0	OAS-CAA	-2.12	1.39	1.43
57	1A	4098	DI0	CBV-CBB	-2.02	1.48	1.53

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	1A	4098	DI0	OBK-CAN-CBQ	-5.60	101.59	110.92
57	1A	4098	DI0	CCA-CBG-CBD	-5.51	104.75	113.40
57	1A	4098	DI0	CBU-CAZ-CAX	-4.87	104.26	112.57
57	1A	4098	DI0	OAM-CAB-OAU	-4.75	97.41	110.67
57	1A	4098	DI0	CBO-CAI-CAK	-4.59	106.58	112.02
57	1A	4098	DI0	CBY-NBE-CBZ	-4.49	97.12	110.38
57	2A	3846	DI0	CAW-OAL-CAE	-4.33	110.48	118.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	1A	4098	DI0	CBT-CAW-CAD	-4.13	107.36	115.20
57	2A	3846	DI0	CAP-CAH-CAJ	-3.86	108.58	114.05
57	2A	3846	DI0	CBT-CAW-CAD	-3.48	108.61	115.20
57	1A	4098	DI0	CAT-CAN-CAX	3.46	113.87	107.67
57	1A	4098	DI0	CBZ-NBE-CAO	-3.42	102.82	113.11
57	1A	4098	DI0	CBD-CAO-NBE	-3.32	106.28	115.67
57	2A	3846	DI0	OBK-CAN-CAX	3.25	108.63	103.81
57	2A	3846	DI0	CBV-CBB-CBC	-3.22	105.13	112.45
57	1A	4098	DI0	OBK-CAN-CAX	3.19	108.54	103.81
57	1A	4098	DI0	OAY-CAR-OAV	-2.90	100.48	109.86
57	2A	3846	DI0	CBO-CAI-CAK	-2.89	108.59	112.02
57	1A	4098	DI0	OBW-CBS-CBA	-2.88	102.77	109.31
57	2A	3846	DI0	CCA-CBG-CBD	-2.81	108.98	113.40
57	1A	4098	DI0	OAS-CAA-CAI	-2.77	104.57	109.99
57	2A	3846	DI0	CAN-CAT-CAR	-2.76	110.29	115.07
57	1A	4098	DI0	CBQ-CAN-CAT	-2.71	105.65	110.49
57	1A	4098	DI0	OBL-CAX-CAZ	-2.69	104.67	109.39
57	2A	3846	DI0	CBD-CAO-NBE	-2.68	108.10	115.67
57	2A	3846	DI0	CBP-CAJ-CAC	-2.62	106.70	111.40
57	2A	3846	DI0	CBM-CAD-CAW	-2.58	107.67	111.31
57	1A	4098	DI0	CBM-CAD-CAW	-2.57	107.69	111.31
57	1A	4098	DI0	OBJ-CAP-CAH	2.52	112.36	107.59
57	1A	4098	DI0	OBH-CAD-CAW	2.41	111.16	107.28
57	1A	4098	DI0	CAR-OAV-CAZ	2.37	120.23	113.84
57	2A	3846	DI0	OAL-CAE-CAF	2.32	116.66	111.56
57	1A	4098	DI0	CAB-OAU-CBG	2.31	116.57	112.91
57	1A	4098	DI0	OBK-CAN-CAT	2.31	116.66	112.96
57	2A	3846	DI0	OAM-CAH-CAP	2.26	109.18	106.39
57	1A	4098	DI0	CBP-CAJ-CAC	-2.24	107.38	111.40
57	2A	3846	DI0	CAR-OAY-CAC	-2.23	110.14	114.66
57	1A	4098	DI0	OAY-CAR-CAT	-2.20	105.21	109.01
57	2A	3846	DI0	CCB-OBK-CAN	-2.20	112.95	117.55
57	1A	4098	DI0	OBJ-CAP-CBR	-2.02	103.81	108.47

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	1A	4098	DI0	CAT-CAN-OBK-CCB
57	1A	4098	DI0	CBR-CAP-CBC-CBB
57	2A	3846	DI0	CBR-CAP-CBC-CBB
57	1A	4098	DI0	CBD-CAO-NBE-CBY

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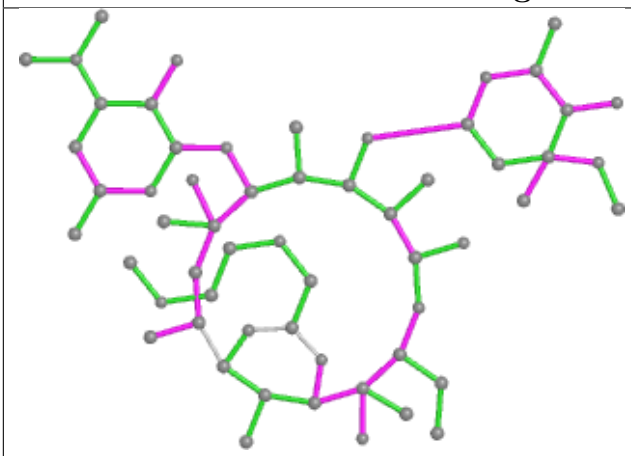
Mol	Chain	Res	Type	Atoms
57	2A	3846	DI0	CBD-CAO-NBE-CBY
57	2A	3846	DI0	CAJ-CAH-CAP-OBJ
57	1A	4098	DI0	OAL-CAW-CBT-CCF
57	2A	3846	DI0	CCC-CCD-OBW-CBS
57	1A	4098	DI0	CBV-CBB-CBC-CAP
57	1A	4098	DI0	NAQ-CBA-CBS-OBW
57	2A	3846	DI0	OAL-CAW-CBT-CCF
57	1A	4098	DI0	OAS-CBA-CBS-OBW
57	1A	4098	DI0	CAJ-CAH-CAP-OBJ
57	1A	4098	DI0	OBJ-CAP-CBC-CBB
57	2A	3846	DI0	OBJ-CAP-CBC-CBB
57	1A	4098	DI0	CAD-CAW-CBT-CCF
57	2A	3846	DI0	CAD-CAW-CBT-CCF
57	2A	3846	DI0	NAQ-CAK-CBB-CBV
57	2A	3846	DI0	NAQ-CAK-CBB-CBC
57	2A	3846	DI0	CAG-CAO-NBE-CBZ

There are no ring outliers.

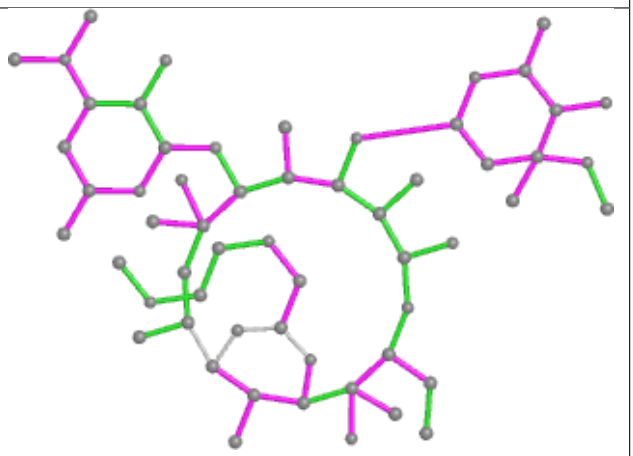
No monomer is involved in short contacts.

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.

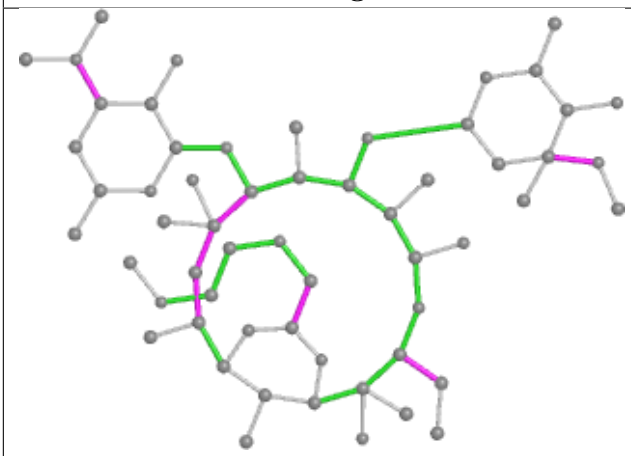
Ligand DI0 1A 4098



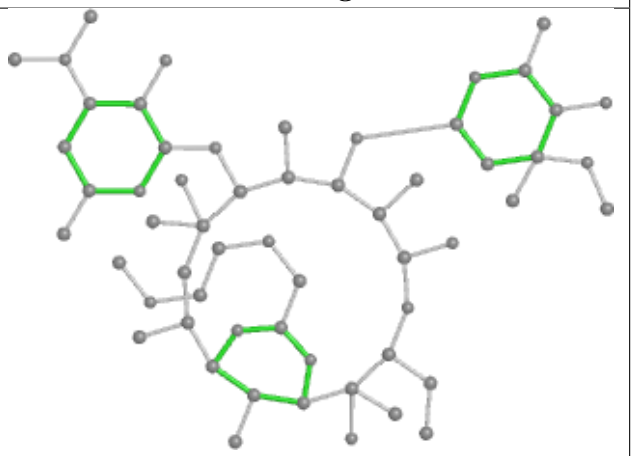
Bond lengths



Bond angles

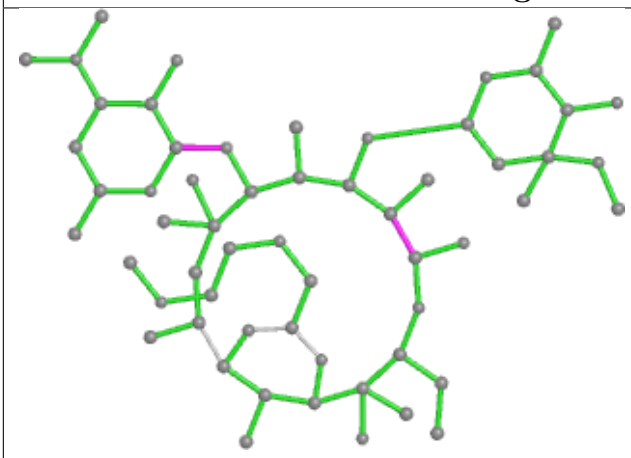


Torsions

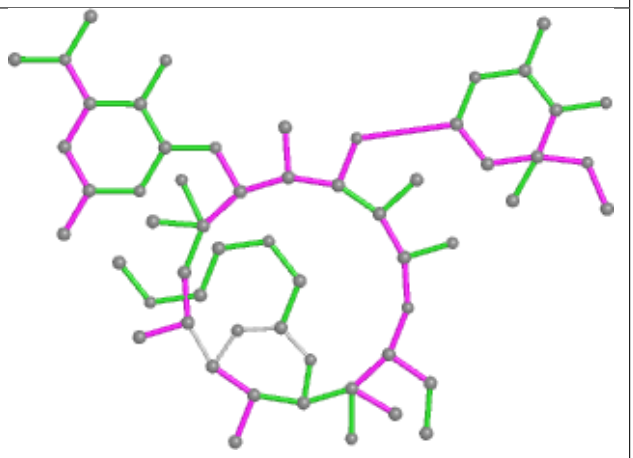


Rings

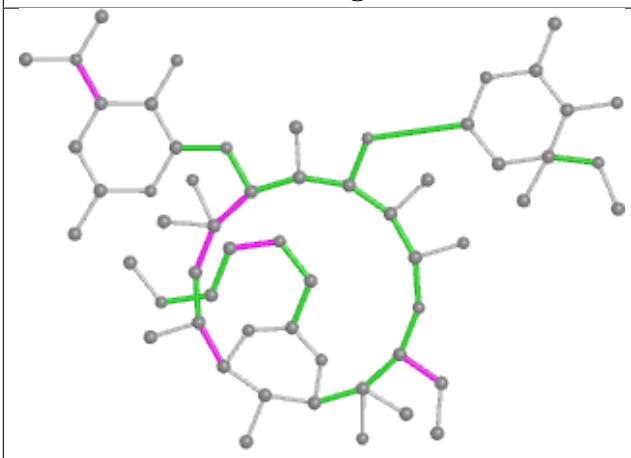
Ligand DI0 2A 3846



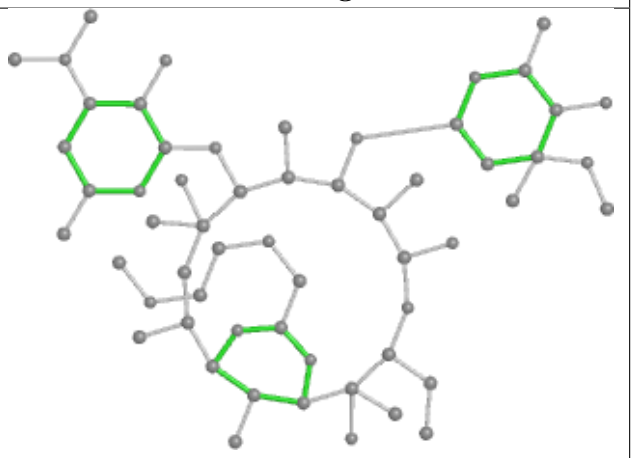
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	0.38	23 (0%) 86 81	18, 35, 99, 114	0
1	2A	2789/2915 (95%)	0.30	28 (1%) 82 77	30, 56, 97, 114	0
2	1B	120/121 (99%)	0.12	0 100 100	28, 48, 63, 92	0
2	2B	120/121 (99%)	-0.03	0 100 100	62, 77, 88, 98	0
3	1D	275/276 (99%)	0.43	2 (0%) 87 84	20, 35, 50, 87	0
3	2D	275/276 (99%)	0.73	10 (3%) 42 32	31, 47, 64, 83	0
4	1E	204/206 (99%)	0.41	4 (1%) 65 56	21, 40, 59, 79	0
4	2E	204/206 (99%)	0.68	13 (6%) 19 12	33, 58, 73, 86	0
5	1F	203/210 (96%)	0.34	2 (0%) 82 77	20, 41, 71, 89	0
5	2F	203/210 (96%)	0.62	9 (4%) 34 24	35, 66, 82, 94	0
6	1G	181/182 (99%)	0.32	1 (0%) 89 86	40, 59, 76, 86	0
6	2G	181/182 (99%)	0.76	22 (12%) 4 2	70, 81, 90, 102	0
7	1H	174/180 (96%)	0.39	3 (1%) 70 63	38, 53, 68, 74	0
7	2H	174/180 (96%)	0.88	27 (15%) 2 1	70, 84, 94, 98	0
8	1I	146/148 (98%)	0.18	0 100 100	40, 73, 82, 88	0
8	2I	146/148 (98%)	0.30	6 (4%) 37 27	54, 72, 85, 90	0
9	1N	140/140 (100%)	0.47	1 (0%) 87 84	27, 37, 62, 74	0
9	2N	140/140 (100%)	1.15	25 (17%) 1 1	45, 64, 81, 85	0
10	1O	122/122 (100%)	0.60	3 (2%) 57 47	26, 38, 56, 65	0
10	2O	122/122 (100%)	0.80	8 (6%) 18 11	42, 57, 71, 78	0
11	1P	149/150 (99%)	0.36	2 (1%) 77 72	20, 45, 73, 84	0
11	2P	149/150 (99%)	0.80	10 (6%) 17 10	34, 69, 83, 94	0
12	1Q	141/141 (100%)	0.64	7 (4%) 28 19	25, 40, 56, 76	0
12	2Q	141/141 (100%)	1.04	17 (12%) 4 2	46, 66, 78, 84	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	1R	118/118 (100%)	0.51	1 (0%) 86 81	23, 33, 48, 59	0
13	2R	118/118 (100%)	0.64	5 (4%) 36 26	39, 51, 62, 73	0
14	1S	110/112 (98%)	0.49	2 (1%) 68 61	35, 48, 61, 66	0
14	2S	110/112 (98%)	0.54	6 (5%) 25 16	62, 72, 82, 85	0
15	1T	131/146 (89%)	0.42	2 (1%) 73 68	30, 43, 71, 80	0
15	2T	131/146 (89%)	0.65	2 (1%) 73 68	52, 61, 80, 87	0
16	1U	116/118 (98%)	0.48	1 (0%) 84 80	22, 30, 49, 63	0
16	2U	116/118 (98%)	0.70	3 (2%) 56 46	42, 61, 76, 84	0
17	1V	101/101 (100%)	0.07	0 100 100	25, 39, 55, 68	0
17	2V	101/101 (100%)	0.61	5 (4%) 28 19	42, 71, 83, 90	0
18	1W	112/113 (99%)	0.60	3 (2%) 54 44	22, 31, 52, 84	0
18	2W	112/113 (99%)	1.23	24 (21%) 0 0	39, 47, 69, 89	0
19	1X	95/96 (98%)	0.42	1 (1%) 80 75	20, 38, 61, 75	0
19	2X	95/96 (98%)	0.73	8 (8%) 11 5	41, 58, 73, 80	0
20	1Y	107/110 (97%)	0.61	4 (3%) 41 31	34, 49, 70, 81	0
20	2Y	107/110 (97%)	1.54	32 (29%) 0 0	59, 72, 83, 89	0
21	1Z	154/206 (74%)	0.88	25 (16%) 1 1	44, 66, 92, 100	0
21	2Z	160/206 (77%)	1.18	38 (23%) 0 0	64, 85, 100, 105	0
22	10	83/85 (97%)	0.81	6 (7%) 15 8	25, 36, 54, 74	0
22	20	83/85 (97%)	0.87	8 (9%) 8 4	45, 62, 73, 86	0
23	11	97/98 (98%)	0.75	2 (2%) 63 54	27, 43, 72, 76	0
23	21	97/98 (98%)	1.01	9 (9%) 8 4	35, 53, 77, 85	0
24	12	70/72 (97%)	0.54	3 (4%) 35 25	35, 46, 59, 81	0
24	22	70/72 (97%)	0.57	2 (2%) 51 41	55, 69, 80, 81	0
25	13	59/60 (98%)	0.23	1 (1%) 70 63	25, 34, 59, 79	0
25	23	59/60 (98%)	0.89	9 (15%) 2 1	49, 66, 82, 90	0
26	14	69/71 (97%)	0.35	2 (2%) 51 41	53, 73, 91, 98	0
26	24	69/71 (97%)	0.43	8 (11%) 4 2	80, 88, 97, 103	0
27	15	59/60 (98%)	0.45	1 (1%) 70 63	19, 31, 48, 67	0
27	25	59/60 (98%)	0.74	1 (1%) 70 63	36, 51, 66, 77	0
28	16	53/54 (98%)	0.34	2 (3%) 40 30	28, 40, 53, 62	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	26	53/54 (98%)	0.63	4 (7%) 14 8	50, 60, 72, 76	0
29	17	48/49 (97%)	0.67	5 (10%) 6 3	21, 27, 55, 64	0
29	27	48/49 (97%)	1.29	9 (18%) 1 1	31, 37, 64, 71	0
30	18	64/65 (98%)	0.62	0 100 100	26, 33, 43, 58	0
30	28	64/65 (98%)	1.03	10 (15%) 2 1	43, 54, 62, 70	0
31	19	37/37 (100%)	0.75	1 (2%) 54 44	30, 39, 59, 61	0
31	29	37/37 (100%)	1.42	10 (27%) 0 0	59, 67, 78, 79	0
32	1a	1488/1521 (97%)	0.22	8 (0%) 91 88	31, 63, 95, 110	0
32	2a	1491/1521 (98%)	0.18	12 (0%) 86 81	49, 77, 99, 114	0
33	1b	231/256 (90%)	0.27	7 (3%) 50 40	61, 80, 93, 96	0
33	2b	231/256 (90%)	1.31	61 (26%) 0 0	74, 89, 97, 102	0
34	1c	206/239 (86%)	0.47	13 (6%) 20 12	56, 69, 83, 91	0
34	2c	206/239 (86%)	0.84	44 (21%) 0 0	76, 86, 93, 99	0
35	1d	208/209 (99%)	1.04	33 (15%) 1 1	51, 66, 79, 87	0
35	2d	208/209 (99%)	1.49	57 (27%) 0 0	63, 73, 84, 89	0
36	1e	148/162 (91%)	0.81	12 (8%) 12 6	49, 63, 75, 87	0
36	2e	148/162 (91%)	1.14	33 (22%) 0 0	68, 78, 87, 90	0
37	1f	100/101 (99%)	0.57	7 (7%) 16 9	50, 65, 76, 81	0
37	2f	100/101 (99%)	0.07	0 100 100	55, 68, 79, 81	0
38	1g	155/156 (99%)	0.26	10 (6%) 18 11	56, 70, 87, 93	0
38	2g	155/156 (99%)	0.61	18 (11%) 4 2	71, 79, 90, 94	0
39	1h	137/138 (99%)	0.27	5 (3%) 42 32	52, 65, 72, 78	0
39	2h	137/138 (99%)	0.58	10 (7%) 15 8	67, 79, 85, 90	0
40	1i	127/128 (99%)	0.43	10 (7%) 12 7	50, 77, 86, 89	0
40	2i	127/128 (99%)	1.64	43 (33%) 0 0	76, 86, 93, 98	0
41	1j	97/105 (92%)	0.61	7 (7%) 15 8	52, 77, 92, 99	0
41	2j	96/105 (91%)	1.12	24 (25%) 0 0	79, 89, 96, 102	0
42	1k	114/129 (88%)	0.48	2 (1%) 68 61	43, 64, 77, 85	0
42	2k	114/129 (88%)	0.58	5 (4%) 34 24	51, 72, 83, 89	0
43	1l	121/132 (91%)	0.38	4 (3%) 46 36	39, 50, 65, 71	0
43	2l	121/132 (91%)	1.12	21 (17%) 1 1	50, 67, 77, 83	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	1m	123/126 (97%)	0.62	7 (5%) 23 15	56, 69, 81, 101	0
44	2m	122/126 (96%)	1.09	23 (18%) 1 1	72, 84, 90, 101	0
45	1n	60/61 (98%)	0.67	2 (3%) 46 36	54, 66, 73, 76	0
45	2n	60/61 (98%)	2.33	29 (48%) 0 0	75, 86, 91, 95	0
46	1o	88/89 (98%)	0.51	2 (2%) 60 51	47, 62, 74, 77	0
46	2o	88/89 (98%)	0.47	3 (3%) 45 35	58, 71, 81, 90	0
47	1p	82/88 (93%)	0.91	10 (12%) 4 2	57, 66, 78, 84	0
47	2p	82/88 (93%)	0.94	11 (13%) 3 1	60, 68, 78, 82	0
48	1q	99/105 (94%)	0.60	5 (5%) 28 19	51, 65, 76, 82	0
48	2q	99/105 (94%)	1.02	15 (15%) 2 1	60, 73, 81, 85	0
49	1r	68/88 (77%)	0.38	1 (1%) 73 68	53, 64, 76, 78	0
49	2r	68/88 (77%)	0.21	0 100 100	58, 71, 84, 89	0
50	1s	83/93 (89%)	0.10	2 (2%) 59 49	59, 72, 83, 86	0
50	2s	83/93 (89%)	1.01	18 (21%) 0 0	81, 89, 96, 99	0
51	1t	96/106 (90%)	0.62	7 (7%) 15 8	57, 69, 81, 85	0
51	2t	96/106 (90%)	0.69	10 (10%) 6 3	61, 70, 84, 86	0
52	1u	23/27 (85%)	1.69	8 (34%) 0 0	59, 64, 74, 75	0
52	2u	23/27 (85%)	1.79	10 (43%) 0 0	77, 82, 87, 90	0
53	1v	13/27 (48%)	1.50	4 (30%) 0 0	45, 56, 94, 105	0
53	2v	13/27 (48%)	1.76	6 (46%) 0 0	63, 82, 101, 101	0
54	1w	67/76 (88%)	0.55	6 (8%) 9 5	41, 90, 101, 106	0
54	1y	67/76 (88%)	0.68	6 (8%) 9 5	35, 101, 108, 112	0
54	2w	67/76 (88%)	1.10	15 (22%) 0 0	55, 99, 105, 111	0
54	2y	67/76 (88%)	0.78	8 (11%) 4 2	53, 103, 107, 110	0
55	1x	72/77 (93%)	0.24	1 (1%) 75 70	36, 69, 89, 93	0
55	2x	72/77 (93%)	0.11	0 100 100	51, 81, 94, 102	0
All	All	20878/21754 (95%)	0.52	1133 (5%) 25 17	18, 62, 93, 114	0

All (1133) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
44	1m	124	PRO	19.3
44	2m	124	PRO	18.6

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Mol	Chain	Res	Type	RSRZ
44	2m	123	ALA	16.7
44	1m	123	ALA	14.3
44	2m	122	LYS	13.9
23	21	2	SER	8.8
45	2n	25	VAL	8.5
38	2g	82	GLY	8.1
33	2b	165	VAL	8.1
45	2n	34	TYR	8.1
21	2Z	170	THR	7.9
45	2n	39	LEU	7.5
3	1D	276	LYS	7.5
35	2d	167	GLY	7.2
54	2w	56	C	7.2
21	2Z	149	SER	6.8
23	11	98	LEU	6.6
27	15	60	VAL	6.5
9	2N	8	GLN	6.3
35	2d	164	ALA	6.3
54	1w	56	C	6.1
31	29	37	GLY	6.1
21	2Z	144	LEU	6.0
44	2m	102	ARG	6.0
33	2b	187	LEU	5.9
38	1g	84	ASN	5.9
40	2i	125	TYR	5.8
41	2j	47	PHE	5.7
29	27	1	MET	5.7
38	2g	79	ARG	5.6
52	2u	14	TRP	5.6
21	1Z	149	SER	5.5
41	2j	59	SER	5.5
20	2Y	45	VAL	5.5
41	2j	58	ASP	5.5
44	2m	121	LYS	5.5
38	2g	80	VAL	5.4
35	2d	168	ARG	5.3
34	2c	196	LEU	5.3
40	2i	110	GLU	5.3
21	1Z	168	GLU	5.3
41	2j	62	HIS	5.2
44	2m	7	VAL	5.2
38	1g	79	ARG	5.1

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Mol	Chain	Res	Type	RSRZ
6	2G	28	VAL	5.1
22	10	6	GLY	5.1
23	11	2	SER	5.0
20	2Y	106	LEU	5.0
35	2d	161	ASN	5.0
35	2d	166	LYS	5.0
33	2b	101	MET	4.9
20	2Y	1	MET	4.9
34	2c	155	GLY	4.9
22	10	3	HIS	4.8
21	2Z	155	LEU	4.8
34	2c	198	VAL	4.8
45	2n	36	PHE	4.8
18	2W	112	GLY	4.8
41	2j	66	ARG	4.7
42	2k	25	TYR	4.7
22	10	5	LYS	4.7
19	2X	92	LEU	4.7
8	2I	85	GLU	4.7
50	2s	79	THR	4.7
41	2j	55	LYS	4.7
44	1m	122	LYS	4.6
26	24	49	PHE	4.6
45	2n	41	ARG	4.5
33	2b	152	PHE	4.5
32	2a	1030(B)	C	4.5
40	2i	9	ARG	4.5
1	2A	888	C	4.5
6	2G	146	TYR	4.5
3	2D	38	LYS	4.5
40	2i	7	THR	4.5
35	2d	160	GLN	4.4
22	10	7	LEU	4.4
40	2i	127	LYS	4.4
40	2i	4	TYR	4.4
41	2j	65	LEU	4.4
38	2g	81	GLY	4.4
24	22	1	MET	4.3
40	2i	102	LEU	4.3
44	2m	120	LYS	4.3
38	2g	4	ARG	4.3
33	2b	215	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
29	27	48	LYS	4.3
45	2n	37	PHE	4.3
12	2Q	103	MET	4.3
12	2Q	104	PHE	4.3
40	2i	115	GLY	4.2
29	17	48	LYS	4.2
33	2b	70	PHE	4.2
38	1g	80	VAL	4.2
20	2Y	63	LYS	4.2
20	2Y	62	GLU	4.2
34	2c	197	GLY	4.2
41	2j	46	ARG	4.2
35	1d	135	LEU	4.2
22	20	2	ALA	4.1
50	2s	80	TYR	4.1
33	2b	48	MET	4.1
6	2G	2	PRO	4.1
41	2j	63	PHE	4.1
43	2l	64	TYR	4.1
40	2i	14	VAL	4.1
21	1Z	170	THR	4.1
50	2s	82	GLY	4.0
36	2e	109	ILE	4.0
53	2v	23	U	4.0
21	2Z	96	VAL	4.0
1	2A	2896	C	4.0
41	2j	48	THR	4.0
29	27	47	ARG	4.0
16	1U	117	GLN	4.0
1	1A	896	A	4.0
43	2l	28	LYS	4.0
23	21	98	LEU	4.0
26	24	54	GLY	4.0
44	2m	119	GLY	4.0
40	2i	81	ILE	4.0
3	2D	276	LYS	4.0
35	2d	152	SER	4.0
35	2d	112	VAL	4.0
50	2s	84	GLY	4.0
36	2e	45	PHE	4.0
22	20	7	LEU	4.0
1	2A	2897	U	4.0

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Mol	Chain	Res	Type	RSRZ
34	2c	4	LYS	4.0
33	2b	135	GLN	4.0
9	2N	9	VAL	3.9
21	2Z	148	ASP	3.9
34	2c	199	LYS	3.9
43	2l	32	PHE	3.9
33	2b	163	PHE	3.9
40	1i	8	GLY	3.9
21	2Z	147	GLY	3.9
53	2v	24	C	3.9
45	2n	57	ARG	3.9
45	2n	42	ILE	3.9
34	2c	160	ALA	3.9
36	2e	22	GLY	3.8
54	2w	71	C	3.8
15	2T	1	MET	3.8
40	2i	114	TYR	3.8
45	2n	58	LYS	3.8
9	2N	45	ASN	3.8
21	2Z	139	VAL	3.8
22	20	3	HIS	3.8
44	2m	6	GLY	3.8
45	2n	22	THR	3.8
45	2n	38	GLY	3.8
52	2u	11	GLY	3.8
21	2Z	125	LEU	3.8
33	2b	34	ALA	3.8
44	2m	4	ILE	3.8
49	1r	78	LEU	3.8
34	2c	14	ILE	3.8
40	2i	109	VAL	3.8
35	1d	157	LEU	3.8
33	2b	31	TYR	3.8
38	2g	156	TRP	3.8
54	2y	36	C	3.8
36	2e	13	ILE	3.8
21	2Z	53	ILE	3.7
35	2d	33	MET	3.7
35	2d	98	GLU	3.7
7	2H	159	GLU	3.7
34	2c	206	GLU	3.7
29	17	47	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
40	2i	119	ALA	3.7
39	2h	83	ILE	3.7
46	1o	87	ILE	3.7
20	2Y	65	ALA	3.7
33	2b	188	ALA	3.7
35	1d	111	ALA	3.7
26	14	55	ARG	3.7
35	2d	146	ILE	3.7
32	1a	1257	U	3.7
4	2E	115	GLY	3.7
35	2d	68	TYR	3.7
6	2G	152	LEU	3.7
36	2e	12	LEU	3.7
20	2Y	60	PHE	3.7
34	2c	193	TYR	3.7
40	2i	36	TYR	3.7
26	24	56	VAL	3.7
34	1c	87	LEU	3.7
21	1Z	121	HIS	3.6
36	2e	17	ALA	3.6
30	28	29	LYS	3.6
35	1d	120	LEU	3.6
40	2i	8	GLY	3.6
45	2n	61	TRP	3.6
34	2c	200	ALA	3.6
26	14	54	GLY	3.6
45	2n	49	HIS	3.6
54	2w	31	C	3.6
12	2Q	1	MET	3.6
40	2i	15	ALA	3.6
50	2s	83	HIS	3.6
33	2b	71	VAL	3.5
35	1d	110	PHE	3.5
35	2d	165	MET	3.5
21	2Z	141	VAL	3.5
51	2t	9	ASN	3.5
18	2W	38	TYR	3.5
45	2n	29	ARG	3.5
21	1Z	169	GLU	3.5
35	2d	20	TYR	3.5
35	1d	167	GLY	3.5
29	27	45	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
33	2b	197	VAL	3.5
35	1d	158	ILE	3.5
38	1g	83	ALA	3.5
33	2b	214	ILE	3.5
34	2c	124	ILE	3.5
20	2Y	54	LYS	3.5
29	27	23	ARG	3.5
35	2d	176	LEU	3.5
6	2G	181	ARG	3.5
35	2d	148	VAL	3.5
32	1a	1531	A	3.5
35	2d	49	ARG	3.4
31	19	26	ILE	3.4
40	2i	62	TYR	3.4
47	2p	19	ILE	3.4
1	1A	1509	C	3.4
45	2n	31	ARG	3.4
40	2i	63	ILE	3.4
35	1d	102	ASP	3.4
9	2N	85	ILE	3.4
33	2b	205	ASP	3.4
35	1d	179	GLU	3.4
39	1h	2	LEU	3.4
44	1m	121	LYS	3.4
21	2Z	126	VAL	3.4
35	1d	3	ARG	3.4
12	2Q	6	ARG	3.4
33	2b	97	TRP	3.4
44	2m	90	LEU	3.4
51	2t	13	LEU	3.4
53	1v	24	C	3.4
21	2Z	57	ILE	3.4
40	2i	106	ALA	3.4
3	2D	5	LYS	3.4
34	2c	2	GLY	3.4
33	2b	210	SER	3.4
34	2c	159	GLY	3.4
36	2e	90	VAL	3.4
21	1Z	102	LEU	3.3
50	2s	71	LEU	3.3
18	2W	20	VAL	3.3
31	29	9	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
35	2d	188	LEU	3.3
53	2v	14	A	3.3
12	2Q	66	ILE	3.3
29	27	46	VAL	3.3
38	1g	81	GLY	3.3
32	2a	1257	U	3.3
54	1y	47	U	3.3
19	2X	68	ARG	3.3
11	2P	45	LEU	3.3
41	2j	49	VAL	3.3
7	2H	29	PRO	3.3
8	2I	1	MET	3.3
51	1t	9	ASN	3.3
21	2Z	122	ARG	3.3
52	2u	10	ARG	3.3
1	1A	1095	A	3.3
1	2A	2802	G	3.3
47	1p	49	LEU	3.3
43	2l	88	GLY	3.3
25	23	60	GLU	3.3
31	29	16	VAL	3.3
36	2e	16	THR	3.3
52	1u	14	TRP	3.3
35	1d	204	ILE	3.2
20	2Y	46	LYS	3.2
33	2b	211	ILE	3.2
43	2l	18	VAL	3.2
52	2u	17	THR	3.2
35	1d	2	GLY	3.2
44	2m	66	LEU	3.2
51	2t	20	LEU	3.2
35	1d	70	ILE	3.2
3	2D	37	LEU	3.2
45	2n	50	LYS	3.2
34	2c	158	GLY	3.2
54	2y	2	G	3.2
41	2j	40	LEU	3.2
35	2d	158	ILE	3.2
40	1i	115	GLY	3.2
39	2h	112	LEU	3.2
1	1A	1093	G	3.2
1	2A	2155	G	3.2

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Mol	Chain	Res	Type	RSRZ
12	2Q	63	LYS	3.2
7	2H	107	VAL	3.2
41	2j	56	HIS	3.2
34	2c	28	GLN	3.2
39	2h	131	GLY	3.2
33	2b	185	ILE	3.2
20	2Y	5	MET	3.2
36	2e	31	LEU	3.2
30	28	16	ILE	3.2
1	2A	896	A	3.2
32	2a	1030(A)	G	3.2
17	2V	42	GLY	3.2
40	1i	114	TYR	3.2
47	1p	59	TRP	3.2
43	2l	7	ILE	3.1
33	2b	94	ASN	3.1
52	2u	22	ARG	3.1
1	2A	2803	C	3.1
44	1m	120	LYS	3.1
42	2k	117	ASN	3.1
44	2m	23	TYR	3.1
33	2b	17	PHE	3.1
36	1e	134	ALA	3.1
54	1y	56	C	3.1
54	2w	61	C	3.1
15	2T	99	LEU	3.1
33	2b	69	LEU	3.1
41	1j	89	ASP	3.1
53	1v	14	A	3.1
9	2N	44	PRO	3.1
25	23	6	VAL	3.1
34	2c	13	GLY	3.1
50	2s	68	GLY	3.1
33	2b	233	SER	3.1
33	2b	164	VAL	3.1
47	1p	7	ALA	3.1
7	2H	71	LEU	3.1
35	2d	78	LEU	3.1
6	2G	39	ILE	3.1
20	2Y	61	ILE	3.1
51	2t	30	LYS	3.1
11	2P	109	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
22	10	2	ALA	3.1
41	2j	64	GLU	3.1
43	2l	68	ALA	3.1
38	2g	16	LEU	3.1
34	1c	193	TYR	3.1
21	1Z	165	VAL	3.1
40	2i	53	VAL	3.1
14	2S	11	LYS	3.1
40	1i	113	LYS	3.1
54	2y	66	A	3.1
21	2Z	121	HIS	3.1
21	2Z	140	ASP	3.1
38	2g	154	TYR	3.1
17	2V	71	LEU	3.0
37	1f	46	ARG	3.0
20	2Y	43	ASN	3.0
33	2b	37	ASN	3.0
41	2j	53	PRO	3.0
1	1A	614(B)	G	3.0
50	2s	38	SER	3.0
9	2N	51	PHE	3.0
30	28	61	LEU	3.0
36	2e	24	ARG	3.0
41	2j	54	PHE	3.0
45	2n	51	GLY	3.0
43	2l	55	VAL	3.0
12	2Q	65	PHE	3.0
45	2n	44	LEU	3.0
45	2n	11	LYS	3.0
1	2A	884	C	3.0
9	2N	43	THR	3.0
33	2b	123	ALA	3.0
35	2d	185	PHE	3.0
9	2N	12	ARG	3.0
38	1g	85	TYR	3.0
47	2p	74	LEU	3.0
48	2q	7	THR	3.0
33	2b	40	HIS	3.0
38	1g	153	HIS	3.0
33	2b	26	PRO	3.0
51	2t	26	ASN	3.0
47	2p	9	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
50	2s	30	LEU	3.0
52	1u	17	THR	3.0
53	1v	13	A	3.0
20	2Y	72	VAL	3.0
32	2a	1034	G	3.0
42	1k	25	TYR	3.0
7	2H	105	LEU	3.0
34	1c	12	LEU	3.0
40	2i	124	GLN	3.0
45	2n	6	LEU	3.0
33	2b	114	ARG	3.0
54	2w	19	G	3.0
12	2Q	22	LYS	3.0
21	2Z	124	ILE	3.0
20	2Y	24	VAL	3.0
36	2e	14	ARG	2.9
34	2c	167	TRP	2.9
36	2e	131	ILE	2.9
12	2Q	30	GLY	2.9
23	21	28	GLY	2.9
36	2e	133	TYR	2.9
43	2l	100	ILE	2.9
22	20	4	LYS	2.9
33	2b	130	ARG	2.9
3	2D	2	ALA	2.9
54	1y	1	G	2.9
1	1A	2132	U	2.9
35	2d	19	LEU	2.9
35	2d	108	LEU	2.9
48	1q	36	ILE	2.9
16	2U	90	VAL	2.9
22	20	5	LYS	2.9
26	24	58	ARG	2.9
44	2m	87	TYR	2.9
6	2G	157	ILE	2.9
20	2Y	29	GLU	2.9
34	2c	173	VAL	2.9
9	2N	116	LEU	2.9
12	2Q	37	LEU	2.9
21	1Z	164	ALA	2.9
48	2q	74	LEU	2.9
54	1y	36	C	2.9

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Mol	Chain	Res	Type	RSRZ
34	2c	6	HIS	2.9
38	2g	86	GLN	2.9
1	1A	1096	A	2.9
20	2Y	55	TYR	2.9
48	2q	36	ILE	2.9
9	2N	10	GLU	2.9
12	2Q	2	LEU	2.9
34	2c	154	SER	2.8
32	1a	204	U	2.8
48	2q	30	PRO	2.8
35	2d	107	ARG	2.8
51	2t	83	ARG	2.8
1	1A	1057	A	2.8
1	2A	2801(A)	A	2.8
9	2N	112	LEU	2.8
24	22	60	LEU	2.8
33	2b	122	PHE	2.8
10	2O	18	LYS	2.8
13	2R	101	ALA	2.8
40	2i	66	ARG	2.8
5	2F	172	TRP	2.8
38	2g	84	ASN	2.8
41	1j	60	ARG	2.8
47	1p	19	ILE	2.8
35	2d	169	LYS	2.8
20	2Y	35	TYR	2.8
19	2X	70	LEU	2.8
35	2d	101	LEU	2.8
54	2w	4	U	2.8
31	29	17	ILE	2.8
45	1n	2	ALA	2.8
14	2S	33	LYS	2.8
20	2Y	47	LYS	2.8
18	2W	13	SER	2.8
20	2Y	75	ILE	2.8
48	2q	60	ILE	2.8
34	2c	153	VAL	2.8
36	2e	119	LEU	2.8
41	2j	61	GLU	2.8
1	1A	2141	G	2.8
36	2e	84	PHE	2.8
25	13	60	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
28	26	11	LEU	2.8
45	2n	13	THR	2.8
10	2O	41	ALA	2.8
23	21	56	GLN	2.8
43	2l	56	ALA	2.8
54	2w	1	G	2.8
30	28	2	PRO	2.8
41	2j	50	ILE	2.8
13	2R	69	ASP	2.8
31	29	12	ASP	2.8
36	2e	81	GLU	2.8
6	2G	133	LEU	2.8
21	1Z	171	ILE	2.7
21	2Z	171	ILE	2.7
34	1c	134	ILE	2.7
36	2e	21	ALA	2.7
36	2e	10	MET	2.7
40	2i	121	ARG	2.7
53	1v	23	U	2.7
46	2o	87	ILE	2.7
13	1R	14	SER	2.7
40	2i	17	VAL	2.7
52	1u	6	ARG	2.7
54	1w	70	C	2.7
48	1q	98	LEU	2.7
20	1Y	1	MET	2.7
21	2Z	69	THR	2.7
43	2l	69	TYR	2.7
52	1u	16	GLY	2.7
21	1Z	100	VAL	2.7
35	1d	5	ILE	2.7
52	2u	13	ILE	2.7
21	1Z	123	ASP	2.7
21	1Z	166	SER	2.7
1	2A	614(A)	U	2.7
1	2A	1026	U	2.7
34	1c	152	ILE	2.7
35	1d	166	LYS	2.7
6	2G	136	ARG	2.7
35	1d	122	ARG	2.7
7	2H	133	VAL	2.7
12	2Q	79	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
26	24	50	VAL	2.7
22	20	68	GLU	2.7
32	2a	1357	A	2.7
52	1u	2	GLY	2.7
14	2S	57	LYS	2.7
40	2i	116	LYS	2.7
19	2X	1	MET	2.7
9	2N	73	THR	2.7
27	25	29	THR	2.7
35	1d	168	ARG	2.7
6	2G	137	GLU	2.7
11	2P	1	MET	2.7
11	2P	79	ARG	2.7
38	2g	32	ARG	2.7
38	2g	78	ARG	2.7
40	2i	128	ARG	2.7
45	2n	35	ARG	2.7
4	2E	52	LEU	2.7
11	1P	149	GLU	2.7
29	17	46	VAL	2.7
40	2i	79	LEU	2.7
1	1A	885	C	2.7
44	2m	65	LYS	2.7
7	2H	48	GLY	2.7
7	2H	101	ARG	2.7
1	2A	2132	U	2.6
7	2H	89	ILE	2.6
20	2Y	44	ILE	2.6
21	1Z	124	ILE	2.6
35	2d	70	ILE	2.6
8	2I	38	LEU	2.6
24	12	70	GLN	2.6
35	2d	194	LEU	2.6
1	2A	2146	C	2.6
33	2b	131	PRO	2.6
18	2W	92	ARG	2.6
45	2n	2	ALA	2.6
18	1W	111	HIS	2.6
21	2Z	48	PHE	2.6
9	2N	83	LYS	2.6
29	17	1	MET	2.6
33	2b	133	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
39	1h	83	ILE	2.6
51	1t	14	LYS	2.6
54	2y	63	G	2.6
40	1i	125	TYR	2.6
21	2Z	70	LEU	2.6
35	1d	11	LEU	2.6
43	2l	27	LEU	2.6
3	2D	51	VAL	2.6
33	2b	201	ILE	2.6
34	2c	134	ILE	2.6
4	2E	195	LEU	2.6
54	1y	5	G	2.6
20	2Y	13	VAL	2.6
31	29	25	VAL	2.6
11	2P	78	PRO	2.6
1	2A	885	C	2.6
22	20	69	PHE	2.6
28	16	54	ILE	2.6
7	2H	2	SER	2.6
14	1S	13	ARG	2.6
40	2i	65	VAL	2.6
46	2o	60	VAL	2.6
47	2p	79	VAL	2.6
1	2A	883	G	2.6
41	1j	98	ILE	2.6
10	2O	17	ARG	2.6
6	2G	34	LEU	2.6
54	2w	47	U	2.6
5	1F	89	VAL	2.6
33	2b	92	TYR	2.6
21	1Z	167	PRO	2.6
34	2c	186	PHE	2.6
40	1i	117	HIS	2.6
10	2O	8	LEU	2.6
19	2X	66	LEU	2.6
21	2Z	76	LEU	2.6
4	2E	196	VAL	2.6
21	2Z	172	ALA	2.6
40	2i	37	PHE	2.6
1	1A	1098	A	2.6
6	2G	138	GLN	2.6
7	2H	148	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
50	2s	32	LYS	2.6
6	2G	19	LEU	2.6
32	1a	163	C	2.6
36	2e	19	MET	2.6
40	2i	6	GLY	2.6
20	1Y	92	ASN	2.6
25	23	53	LEU	2.6
36	2e	100	VAL	2.6
39	2h	129	VAL	2.6
41	2j	44	VAL	2.6
54	1w	61	C	2.6
41	2j	60	ARG	2.6
12	2Q	69	PHE	2.6
35	1d	136	PRO	2.6
33	2b	72	GLY	2.5
36	1e	19	MET	2.5
33	2b	19	HIS	2.5
20	2Y	26	LYS	2.5
34	2c	207	VAL	2.5
40	1i	14	VAL	2.5
1	2A	2793	G	2.5
43	2l	22	SER	2.5
33	1b	188	ALA	2.5
48	1q	27	PHE	2.5
21	2Z	150	LEU	2.5
26	24	52	THR	2.5
35	2d	120	LEU	2.5
50	1s	71	LEU	2.5
9	2N	140	VAL	2.5
21	2Z	151	HIS	2.5
36	1e	27	ARG	2.5
48	2q	21	VAL	2.5
26	24	63	TYR	2.5
1	2A	614(B)	G	2.5
44	2m	5	ALA	2.5
54	2y	1	G	2.5
12	2Q	33	GLY	2.5
21	2Z	156	LYS	2.5
36	2e	89	ILE	2.5
11	1P	15	ARG	2.5
9	2N	50	ASP	2.5
1	2A	229	A	2.5

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Mol	Chain	Res	Type	RSRZ
11	2P	110	TYR	2.5
20	2Y	25	GLY	2.5
33	2b	228	GLY	2.5
52	2u	15	ARG	2.5
8	2I	35	LEU	2.5
51	2t	24	LEU	2.5
6	2G	159	VAL	2.5
18	2W	85	VAL	2.5
41	2j	72	VAL	2.5
23	21	81	LYS	2.5
35	2d	179	GLU	2.5
48	2q	100	LYS	2.5
1	1A	2803	C	2.5
32	2a	1116	C	2.5
14	2S	20	ARG	2.5
21	1Z	160	GLY	2.5
34	2c	37	GLN	2.5
34	2c	182	ILE	2.5
34	1c	196	LEU	2.5
4	2E	150	VAL	2.5
4	2E	10	GLY	2.5
6	1G	146	TYR	2.5
34	2c	23	TYR	2.5
6	2G	140	ILE	2.5
28	26	54	ILE	2.5
35	2d	175	SER	2.5
45	2n	60	SER	2.5
3	1D	38	LYS	2.5
7	2H	123	PHE	2.5
40	2i	18	PHE	2.5
41	1j	58	ASP	2.5
26	24	40	HIS	2.5
28	26	2	ALA	2.5
33	1b	77	ALA	2.5
34	2c	184	TYR	2.5
4	1E	195	LEU	2.5
21	1Z	156	LYS	2.5
35	1d	21	LEU	2.5
35	2d	18	LYS	2.5
20	2Y	7	VAL	2.5
21	2Z	162	GLU	2.5
21	2Z	173	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
35	2d	54	TYR	2.5
38	1g	154	TYR	2.5
7	2H	43	VAL	2.5
7	2H	141	VAL	2.5
9	2N	68	GLU	2.5
32	2a	1532	U	2.5
34	2c	190	ARG	2.5
47	1p	25	ARG	2.5
52	1u	22	ARG	2.5
36	2e	86	ALA	2.5
33	2b	196	LEU	2.5
1	1A	884	C	2.4
51	1t	22	ARG	2.4
19	2X	28	PHE	2.4
20	2Y	59	GLY	2.4
34	2c	149	ALA	2.4
41	2j	10	GLY	2.4
43	2l	26	ALA	2.4
34	2c	157	ILE	2.4
44	2m	103	THR	2.4
20	2Y	50	ARG	2.4
44	2m	104	ARG	2.4
6	2G	142	PRO	2.4
43	2l	31	PRO	2.4
25	23	47	VAL	2.4
40	2i	26	VAL	2.4
18	2W	94	ASP	2.4
29	27	22	MET	2.4
33	2b	14	GLY	2.4
38	2g	152	ALA	2.4
34	2c	5	ILE	2.4
46	1o	57	LEU	2.4
35	1d	8	VAL	2.4
35	2d	198	VAL	2.4
12	1Q	80	GLU	2.4
18	2W	6	ILE	2.4
36	2e	47	LYS	2.4
43	1l	7	ILE	2.4
43	1l	91	LYS	2.4
10	2O	81	ASP	2.4
21	2Z	93	ASP	2.4
41	2j	51	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	2A	508	G	2.4
20	1Y	40	GLU	2.4
33	2b	8	LYS	2.4
43	1l	13	LYS	2.4
14	2S	58	LEU	2.4
18	2W	69	LEU	2.4
33	1b	215	LEU	2.4
41	1j	8	LEU	2.4
46	2o	57	LEU	2.4
43	2l	25	PRO	2.4
54	2y	35	A	2.4
5	2F	79	GLY	2.4
23	21	61	ARG	2.4
35	2d	16	GLY	2.4
18	2W	36	LEU	2.4
32	2a	1202	G	2.4
40	2i	19	LEU	2.4
30	28	22	VAL	2.4
36	2e	105	VAL	2.4
35	1d	80	GLU	2.4
40	1i	112	LYS	2.4
53	2v	13	A	2.4
10	1O	108	GLU	2.4
34	2c	8	ILE	2.4
39	2h	134	ILE	2.4
51	2t	22	ARG	2.4
36	1e	82	VAL	2.4
35	1d	62	GLN	2.4
33	2b	77	ALA	2.4
4	2E	181	LEU	2.4
21	2Z	137	ILE	2.4
31	29	15	LYS	2.4
5	2F	57	VAL	2.4
7	2H	45	VAL	2.4
11	2P	149	GLU	2.4
21	2Z	86	VAL	2.4
33	1b	232	PRO	2.4
33	2b	81	VAL	2.4
34	2c	205	GLY	2.4
19	1X	1	MET	2.4
36	2e	125	SER	2.4
38	2g	77	SER	2.4

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Mol	Chain	Res	Type	RSRZ
54	2w	76	A	2.4
33	2b	32	ILE	2.4
32	1a	345	C	2.4
35	2d	23	GLY	2.3
39	1h	93	VAL	2.3
52	2u	16	GLY	2.3
18	2W	9	TYR	2.3
33	2b	79	ASP	2.3
35	2d	3	ARG	2.3
40	1i	106	ALA	2.3
16	2U	44	ASN	2.3
38	1g	156	TRP	2.3
21	1Z	120	ILE	2.3
47	2p	6	LEU	2.3
55	1x	67	C	2.3
35	2d	121	VAL	2.3
19	2X	69	TYR	2.3
34	2c	7	PRO	2.3
35	2d	106	TYR	2.3
12	1Q	5	ARG	2.3
45	2n	12	ARG	2.3
43	2l	60	LEU	2.3
17	2V	43	GLU	2.3
8	2I	3	VAL	2.3
42	1k	13	GLN	2.3
31	29	24	TYR	2.3
35	1d	138	TYR	2.3
40	2i	105	ASP	2.3
7	2H	96	ALA	2.3
21	2Z	51	ALA	2.3
34	2c	189	ALA	2.3
35	2d	2	GLY	2.3
45	2n	55	GLY	2.3
47	1p	35	LYS	2.3
15	1T	108	ARG	2.3
18	2W	47	VAL	2.3
33	2b	140	HIS	2.3
51	2t	25	ARG	2.3
54	2w	32	C	2.3
10	2O	1	MET	2.3
25	23	21	ALA	2.3
28	16	2	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
36	1e	21	ALA	2.3
38	2g	83	ALA	2.3
38	1g	82	GLY	2.3
7	2H	132	ARG	2.3
29	27	41	ARG	2.3
32	1a	162	A	2.3
53	2v	12	A	2.3
12	1Q	79	LEU	2.3
30	28	58	ILE	2.3
48	2q	22	LEU	2.3
35	2d	115	ARG	2.3
47	2p	62	VAL	2.3
33	2b	232	PRO	2.3
47	1p	32	TYR	2.3
47	1p	39	TYR	2.3
54	1w	57	G	2.3
3	2D	204	ILE	2.3
35	1d	101	LEU	2.3
51	1t	24	LEU	2.3
21	1Z	104	PHE	2.3
40	2i	33	PHE	2.3
18	2W	50	VAL	2.3
50	2s	41	VAL	2.3
39	2h	99	GLU	2.3
34	2c	33	LEU	2.3
44	2m	88	ARG	2.3
45	2n	59	ALA	2.3
48	2q	65	ILE	2.3
47	1p	27	LYS	2.3
40	1i	126	SER	2.3
9	2N	119	ARG	2.3
21	1Z	151	HIS	2.3
33	2b	21	ARG	2.3
33	2b	36	ARG	2.3
43	2l	89	ARG	2.3
6	2G	3	LEU	2.3
1	2A	1509	C	2.3
4	1E	1	MET	2.3
21	2Z	91	LEU	2.3
39	1h	10	LEU	2.3
20	2Y	89	PHE	2.3
54	1y	21	A	2.3

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Mol	Chain	Res	Type	RSRZ
7	2H	113	VAL	2.2
18	2W	17	VAL	2.2
34	1c	126	ARG	2.2
10	1O	122	LEU	2.2
12	1Q	41	TRP	2.2
18	2W	1	MET	2.2
30	28	34	TRP	2.2
31	29	1	MET	2.2
33	2b	227	GLY	2.2
35	1d	19	LEU	2.2
1	1A	889	C	2.2
12	2Q	32	TYR	2.2
51	1t	18	GLN	2.2
4	2E	116	VAL	2.2
12	1Q	81	VAL	2.2
32	1a	344	A	2.2
21	1Z	122	ARG	2.2
35	2d	47	ARG	2.2
36	2e	130	ASN	2.2
40	2i	83	ARG	2.2
54	2y	53	G	2.2
1	1A	1026	U	2.2
1	1A	1094	U	2.2
36	2e	9	LYS	2.2
21	2Z	163	LEU	2.2
40	2i	117	HIS	2.2
4	2E	151	TYR	2.2
34	2c	201	TYR	2.2
5	2F	89	VAL	2.2
34	1c	85	ARG	2.2
14	2S	83	LYS	2.2
20	2Y	19	LYS	2.2
7	2H	103	LEU	2.2
43	2l	5	PRO	2.2
44	2m	76	ALA	2.2
47	2p	33	ILE	2.2
5	2F	62	ARG	2.2
47	2p	76	GLN	2.2
52	2u	6	ARG	2.2
1	2A	2794	C	2.2
31	29	13	LYS	2.2
48	2q	11	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
54	2w	72	C	2.2
35	2d	196	LEU	2.2
18	2W	103	ILE	2.2
44	2m	97	PRO	2.2
36	1e	10	MET	2.2
39	2h	84	ARG	2.2
34	1c	201	TYR	2.2
1	1A	1092	C	2.2
28	26	5	VAL	2.2
40	2i	28	VAL	2.2
21	1Z	150	LEU	2.2
33	2b	186	ALA	2.2
35	2d	141	ARG	2.2
36	1e	25	ARG	2.2
44	2m	42	ALA	2.2
6	2G	29	TRP	2.2
1	2A	2804	C	2.2
33	2b	50	GLU	2.2
35	1d	162	LEU	2.2
36	1e	119	LEU	2.2
37	1f	61	LEU	2.2
47	2p	42	ARG	2.2
5	2F	53	THR	2.2
30	28	10	ALA	2.2
35	2d	48	ALA	2.2
12	1Q	7	MET	2.2
40	2i	49	PRO	2.2
33	1b	165	VAL	2.2
24	12	69	ARG	2.2
52	1u	10	ARG	2.2
54	2y	62	C	2.2
17	2V	39	LEU	2.2
36	2e	110	LEU	2.2
39	2h	2	LEU	2.2
48	2q	98	LEU	2.2
38	2g	2	ALA	2.2
9	2N	1	MET	2.2
33	2b	67	THR	2.2
20	2Y	40	GLU	2.2
20	2Y	81	LYS	2.2
21	2Z	161	VAL	2.2
35	2d	184	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
36	2e	33	VAL	2.2
47	2p	34	GLU	2.2
25	23	27	GLY	2.2
40	2i	16	ARG	2.2
1	1A	2145	C	2.2
5	2F	181	LEU	2.2
13	2R	65	LEU	2.2
32	2a	1066	C	2.2
29	17	45	ALA	2.2
35	2d	5	ILE	2.2
35	2d	32	ALA	2.2
33	2b	90	MET	2.2
9	2N	61	ARG	2.2
11	2P	76	LYS	2.2
25	23	30	ARG	2.2
1	1A	1084	A	2.2
34	1c	198	VAL	2.2
4	2E	6	GLY	2.1
52	1u	18	TYR	2.2
6	2G	7	LEU	2.1
13	2R	10	LEU	2.1
37	1f	21	LEU	2.1
25	23	51	ALA	2.1
33	2b	68	ILE	2.1
51	2t	41	ILE	2.1
54	2w	57	G	2.1
7	1H	18	GLU	2.1
20	2Y	12	THR	2.1
52	2u	9	ARG	2.1
12	2Q	96	VAL	2.1
3	2D	15	PHE	2.1
10	1O	91	LEU	2.1
17	2V	75	PHE	2.1
35	2d	110	PHE	2.1
41	1j	40	LEU	2.1
6	2G	41	GLN	2.1
18	2W	81	ALA	2.1
33	2b	218	ALA	2.1
35	1d	201	GLN	2.1
50	1s	40	ILE	2.1
1	1A	1100	C	2.1
40	2i	120	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
45	2n	23	ARG	2.1
50	2s	69	HIS	2.1
4	2E	104	VAL	2.1
35	1d	170	VAL	2.1
6	2G	75	LYS	2.1
22	10	4	LYS	2.1
1	2A	2173	A	2.1
3	2D	247	ALA	2.1
5	2F	166	ALA	2.1
9	2N	60	ILE	2.1
18	2W	24	ILE	2.1
34	1c	131	ARG	2.1
34	2c	202	ILE	2.1
35	2d	73	ARG	2.1
36	2e	80	ILE	2.1
44	1m	2	ALA	2.1
50	2s	81	ARG	2.1
7	2H	24	VAL	2.1
33	1b	233	SER	2.1
1	2A	882	G	2.1
33	2b	139	LYS	2.1
4	1E	183	LEU	2.1
30	28	64	TYR	2.1
33	1b	163	PHE	2.1
35	2d	206	PHE	2.1
39	1h	133	LEU	2.1
50	2s	15	LEU	2.1
23	21	75	GLU	2.1
36	1e	89	ILE	2.1
50	2s	49	ILE	2.1
1	2A	886	C	2.1
42	2k	35	PRO	2.1
9	2N	5	VAL	2.1
38	2g	153	HIS	2.1
40	2i	126	SER	2.1
35	2d	118	ARG	2.1
36	2e	98	THR	2.1
7	2H	47	GLU	2.1
9	2N	72	TYR	2.1
21	2Z	145	GLU	2.1
35	2d	157	LEU	2.1
40	2i	5	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
42	2k	50	TYR	2.1
48	2q	32	TYR	2.1
21	2Z	154	ASP	2.1
5	2F	80	ALA	2.1
18	2W	93	ALA	2.1
23	21	29	GLY	2.1
1	1A	2142	C	2.1
37	1f	85	VAL	2.1
3	2D	155	LEU	2.1
5	1F	53	THR	2.1
10	2O	122	LEU	2.1
18	2W	104	THR	2.1
24	12	37	PHE	2.1
37	1f	14	LEU	2.1
4	2E	134	ILE	2.1
45	1n	7	ILE	2.1
54	2w	10	G	2.1
34	2c	171	GLY	2.1
1	1A	890	A	2.1
7	1H	19	VAL	2.1
9	2N	134	ARG	2.1
20	2Y	73	ARG	2.1
35	1d	66	ARG	2.1
35	1d	159	ARG	2.1
35	2d	189	PRO	2.1
47	2p	51	VAL	2.1
50	2s	59	PRO	2.1
33	2b	35	GLU	2.1
9	2N	23	LEU	2.1
13	2R	47	PHE	2.1
30	28	15	LYS	2.1
10	2O	19	ILE	2.1
25	23	25	ALA	2.1
43	2l	85	ILE	2.1
1	2A	2131	G	2.1
7	2H	114	VAL	2.1
12	1Q	1	MET	2.1
32	2a	1061	G	2.1
38	2g	3	ARG	2.1
51	1t	8	ARG	2.1
11	2P	2	LYS	2.1
14	1S	83	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
35	2d	11	LEU	2.1
51	1t	20	LEU	2.1
50	2s	52	TYR	2.1
7	2H	169	VAL	2.1
43	1l	16	GLU	2.1
43	2l	46	LYS	2.1
16	2U	20	LEU	2.0
34	2c	188	LEU	2.0
41	1j	68	HIS	2.0
50	2s	35	SER	2.0
54	1w	71	C	2.0
7	2H	162	ILE	2.0
21	1Z	148	ASP	2.0
18	2W	37	ARG	2.0
19	2X	60	ARG	2.0
33	2b	111	ARG	2.0
33	2b	222	ILE	2.0
44	2m	78	ILE	2.0
7	1H	25	LYS	2.0
9	2N	118	LYS	2.0
48	2q	77	VAL	2.0
21	1Z	163	LEU	2.0
34	2c	204	LEU	2.0
37	1f	60	PHE	2.0
44	1m	19	LEU	2.0
11	2P	50	ARG	2.0
32	2a	973	G	2.0
21	1Z	137	ILE	2.0
36	1e	18	ARG	2.0
42	2k	126	ARG	2.0
41	2j	52	GLY	2.0
47	1p	48	TRP	2.0
53	2v	15	A	2.0
54	1w	72	C	2.0
8	2I	122	GLU	2.0
18	1W	112	GLY	2.0
34	1c	184	TYR	2.0
7	2H	52	VAL	2.0
7	2H	131	VAL	2.0
36	2e	82	VAL	2.0
48	1q	35	VAL	2.0
12	2Q	39	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
18	2W	86	LEU	2.0
34	2c	3	ASN	2.0
35	1d	108	LEU	2.0
35	2d	186	LEU	2.0
18	2W	90	ARG	2.0
34	1c	164	ARG	2.0
48	1q	38	ARG	2.0
7	2H	72	ILE	2.0
9	1N	16	ILE	2.0
18	2W	96	ILE	2.0
36	2e	121	LYS	2.0
1	2A	2154	G	2.0
4	1E	87	GLU	2.0
22	20	8	GLY	2.0
54	2w	28	C	2.0
1	2A	6	A	2.0
32	2a	1092	A	2.0
39	2h	138	TRP	2.0
35	1d	181	MET	2.0
39	2h	9	MET	2.0
6	2G	135	LEU	2.0
21	2Z	82	ARG	2.0
48	2q	26	GLN	2.0
48	2q	78	GLU	2.0
1	1A	888	C	2.0
4	2E	25	VAL	2.0
15	1T	115	ARG	2.0
18	1W	39	THR	2.0
32	1a	1003	G	2.0
54	2w	2	G	2.0
35	2d	209	ARG	2.0
36	1e	24	ARG	2.0
20	1Y	4	LYS	2.0
21	1Z	155	LEU	2.0
23	21	68	PRO	2.0
29	27	2	LYS	2.0
45	2n	16	PHE	2.0
36	1e	123	LEU	2.0
37	1f	16	GLN	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	2w	55	20/21	0.53	0.28	80,102,110,113	0
54	PSU	1w	55	20/21	0.62	0.31	64,91,100,110	0
54	CM0	1y	34	25/26	0.64	0.36	89,95,104,121	0
54	PSU	1y	55	20/21	0.68	0.27	95,103,109,120	0
54	PSU	2y	55	20/21	0.70	0.26	96,103,116,128	0
54	4SU	2y	8	20/21	0.71	0.14	94,102,118,127	0
54	CM0	2y	34	25/26	0.71	0.48	85,101,107,121	0
54	7MG	2y	46	24/25	0.73	0.18	95,105,113,128	0
54	5MU	1y	54	21/22	0.73	0.26	88,98,107,120	0
54	4SU	1y	8	20/21	0.74	0.21	97,103,115,130	0
54	5MU	2y	54	21/22	0.74	0.29	91,100,114,130	0
54	6MZ	1y	37	23/24	0.75	0.23	89,97,110,126	0
54	6MZ	2y	37	23/24	0.77	0.32	92,100,114,137	0
54	7MG	1y	46	24/25	0.80	0.19	88,104,109,121	0
54	4SU	2w	8	20/21	0.80	0.22	91,103,115,116	0
54	7MG	1w	46	24/25	0.84	0.16	83,93,101,112	0
54	5MU	2w	54	21/22	0.85	0.16	81,87,94,98	0
54	7MG	2w	46	24/25	0.85	0.19	87,98,108,119	0
55	4SU	2x	8	20/21	0.87	0.14	78,85,92,96	0
54	4SU	1w	8	20/21	0.88	0.13	84,89,100,104	0
55	PSU	2x	55	20/21	0.89	0.12	75,82,88,93	0
54	5MU	1w	54	21/22	0.90	0.19	57,74,84,89	0
32	2MG	2a	1207	24/25	0.90	0.17	74,89,97,103	0
54	CM0	2w	34	25/26	0.92	0.20	65,79,90,95	0
55	4SU	1x	8	20/21	0.92	0.17	55,64,84,86	0
32	PSU	2a	516	20/21	0.92	0.17	61,75,81,85	0
32	M2G	2a	966	25/26	0.92	0.20	58,66,80,85	0
55	5MC	2x	32	21/22	0.93	0.24	65,72,78,84	0
32	5MC	2a	967	21/22	0.94	0.20	64,70,78,82	0
43	0TD	1l	92	10/11	0.94	0.21	39,46,49,68	0
54	6MZ	2w	37	23/24	0.94	0.25	67,78,83,85	0
55	5MU	2x	54	21/22	0.94	0.15	83,87,89,95	0
43	0TD	2l	92	10/11	0.94	0.35	60,65,68,82	0
32	7MG	2a	527	24/25	0.95	0.22	58,65,72,84	0
1	5MU	1A	1915	21/22	0.95	0.18	51,57,61,65	0
1	5MC	2A	1962	21/22	0.95	0.18	43,50,58,67	0
1	5MU	2A	1915	21/22	0.95	0.17	66,73,79,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	5MC	2A	1942	21/22	0.95	0.16	51,59,66,73	0
32	5MC	2a	1400	21/22	0.95	0.26	60,68,71,76	0
54	CM0	1w	34	25/26	0.95	0.17	49,64,67,70	0
32	4OC	2a	1402	22/23	0.95	0.19	56,62,65,70	0
32	5MC	2a	1404	21/22	0.95	0.19	47,55,64,66	0
55	PSU	1x	55	20/21	0.95	0.15	60,66,75,78	0
32	MA6	2a	1518	24/25	0.95	0.21	49,61,66,66	0
32	PSU	1a	516	20/21	0.96	0.19	52,57,61,61	0
32	7MG	1a	527	24/25	0.96	0.21	38,45,51,54	0
32	MA6	2a	1519	24/25	0.96	0.27	53,59,63,64	0
1	4OC	2A	1920	21/23	0.96	0.17	48,59,64,66	0
55	5MU	1x	54	21/22	0.96	0.15	59,71,76,78	0
1	PSU	2A	1911	20/21	0.96	0.17	57,63,65,75	0
1	PSU	1A	1917	20/21	0.96	0.21	43,49,56,60	0
1	PSU	2A	1917	20/21	0.96	0.15	61,65,74,75	0
32	5MC	1a	1404	21/22	0.97	0.24	32,41,49,51	0
32	5MC	2a	1407	21/22	0.97	0.20	48,54,58,62	0
32	UR3	2a	1498	21/22	0.97	0.22	54,58,63,70	0
1	PSU	2A	2605	20/21	0.97	0.21	30,37,44,45	0
1	OMG	2A	2251	24/25	0.97	0.23	35,40,44,44	0
54	6MZ	1w	37	23/24	0.97	0.22	39,48,57,60	0
1	2MA	2A	2503	23/24	0.97	0.22	28,36,40,41	0
1	PSU	1A	1911	20/21	0.97	0.18	39,49,52,56	0
32	M2G	1a	966	25/26	0.97	0.22	46,50,58,65	0
55	5MC	1x	32	21/22	0.97	0.21	41,54,60,62	0
32	5MC	1a	967	21/22	0.97	0.25	43,50,56,60	0
1	4OC	1A	1920	21/23	0.97	0.19	37,45,50,56	0
32	2MG	1a	1207	24/25	0.97	0.17	59,66,72,74	0
32	5MC	1a	1400	21/22	0.97	0.21	37,50,53,57	0
32	4OC	1a	1402	22/23	0.97	0.22	41,46,52,60	0
1	PSU	1A	2605	20/21	0.98	0.20	22,26,35,35	0
32	MA6	1a	1518	24/25	0.98	0.23	30,38,41,42	0
32	MA6	1a	1519	24/25	0.98	0.23	32,39,42,47	0
1	2MU	2A	2552	21/23	0.98	0.20	35,39,47,49	0
1	5MU	2A	1939	21/22	0.98	0.21	35,38,45,46	0
32	5MC	1a	1407	21/22	0.98	0.21	27,39,42,43	0
1	5MU	1A	1939	21/22	0.98	0.21	20,28,32,37	0
1	5MC	1A	1942	21/22	0.98	0.18	37,42,47,53	0
1	5MC	1A	1962	21/22	0.98	0.19	32,36,42,52	0
1	OMG	1A	2251	24/25	0.98	0.23	19,25,27,29	0
1	2MU	1A	2552	21/23	0.98	0.25	23,27,33,35	0
32	UR3	1a	1498	21/22	0.99	0.25	29,39,43,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	2MA	1A	2503	23/24	0.99	0.24	17,21,25,28	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	1A	3979	1/1	-0.12	0.54	92,92,92,92	0
56	MG	1A	4055	1/1	0.26	0.22	67,67,67,67	0
56	MG	1A	3962	1/1	0.34	0.12	72,72,72,72	0
56	MG	2a	1649	1/1	0.37	0.35	69,69,69,69	0
56	MG	2a	1762	1/1	0.39	0.30	104,104,104,104	0
56	MG	1A	4009	1/1	0.40	0.17	74,74,74,74	0
56	MG	2a	1756	1/1	0.43	0.18	72,72,72,72	0
56	MG	1A	3267	1/1	0.44	0.32	38,38,38,38	0
56	MG	2A	3606	1/1	0.48	0.26	79,79,79,79	0
56	MG	1A	3282	1/1	0.48	0.45	53,53,53,53	0
56	MG	2a	1817	1/1	0.48	0.09	95,95,95,95	0
56	MG	1A	3586	1/1	0.49	0.29	76,76,76,76	0
56	MG	1A	3939	1/1	0.49	0.20	84,84,84,84	0
56	MG	1A	3293	1/1	0.49	0.58	56,56,56,56	0
56	MG	2A	3391	1/1	0.49	0.36	79,79,79,79	0
56	MG	2A	3504	1/1	0.49	0.18	66,66,66,66	0
56	MG	2a	1819	1/1	0.49	0.17	69,69,69,69	0
56	MG	1B	235	1/1	0.50	0.38	81,81,81,81	0
56	MG	2A	3122	1/1	0.51	0.17	73,73,73,73	0
56	MG	2A	3302	1/1	0.52	0.92	61,61,61,61	0
56	MG	2a	1821	1/1	0.52	0.25	72,72,72,72	0
56	MG	2A	3485	1/1	0.53	0.27	61,61,61,61	0
56	MG	15	103	1/1	0.54	0.60	60,60,60,60	0
56	MG	2A	3774	1/1	0.55	0.23	71,71,71,71	0
56	MG	2A	3138	1/1	0.56	0.22	68,68,68,68	0
56	MG	1A	3468	1/1	0.56	0.33	82,82,82,82	0
56	MG	1a	1689	1/1	0.56	0.26	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	2B	202	1/1	0.56	0.34	84,84,84,84	0
56	MG	2A	3340	1/1	0.56	0.25	69,69,69,69	0
56	MG	2a	1697	1/1	0.56	0.17	76,76,76,76	0
56	MG	1A	3477	1/1	0.56	0.36	59,59,59,59	0
56	MG	1A	3529	1/1	0.56	0.18	60,60,60,60	0
56	MG	1A	3223	1/1	0.56	0.65	56,56,56,56	0
56	MG	1A	3848	1/1	0.56	0.63	37,37,37,37	0
56	MG	1A	3918	1/1	0.56	0.13	53,53,53,53	0
56	MG	2A	3678	1/1	0.57	0.13	85,85,85,85	0
56	MG	2a	1804	1/1	0.57	0.46	79,79,79,79	0
56	MG	1A	3502	1/1	0.57	0.48	55,55,55,55	0
56	MG	2a	1741	1/1	0.57	0.10	80,80,80,80	0
56	MG	1A	3914	1/1	0.57	0.11	71,71,71,71	0
56	MG	1A	3975	1/1	0.58	0.10	113,113,113,113	0
56	MG	2a	1793	1/1	0.58	0.13	74,74,74,74	0
56	MG	1A	3982	1/1	0.58	0.15	42,42,42,42	0
56	MG	2A	3056	1/1	0.59	0.35	74,74,74,74	0
56	MG	2a	1624	1/1	0.59	0.66	70,70,70,70	0
56	MG	1A	4097	1/1	0.59	0.13	60,60,60,60	0
56	MG	2A	3552	1/1	0.59	0.12	42,42,42,42	0
56	MG	2a	1815	1/1	0.60	0.21	75,75,75,75	0
56	MG	2A	3332	1/1	0.60	0.56	71,71,71,71	0
56	MG	2A	3411	1/1	0.60	0.54	65,65,65,65	0
56	MG	2a	1659	1/1	0.60	0.12	73,73,73,73	0
56	MG	1a	1833	1/1	0.61	0.11	68,68,68,68	0
56	MG	2a	1743	1/1	0.61	0.09	96,96,96,96	0
56	MG	1A	4003	1/1	0.62	0.28	84,84,84,84	0
56	MG	1A	3548	1/1	0.62	0.20	47,47,47,47	0
56	MG	2a	1671	1/1	0.62	0.18	68,68,68,68	0
56	MG	1A	3347	1/1	0.62	0.24	67,67,67,67	0
56	MG	2A	3668	1/1	0.62	0.16	49,49,49,49	0
56	MG	1A	4061	1/1	0.62	0.25	65,65,65,65	0
56	MG	1A	4081	1/1	0.62	2.45	92,92,92,92	0
56	MG	2a	1625	1/1	0.63	0.51	74,74,74,74	0
56	MG	1A	4017	1/1	0.63	0.13	70,70,70,70	0
56	MG	2a	1652	1/1	0.63	0.28	82,82,82,82	0
56	MG	1A	3594	1/1	0.63	0.32	48,48,48,48	0
56	MG	1A	4050	1/1	0.64	0.13	37,37,37,37	0
56	MG	2A	3136	1/1	0.64	0.18	63,63,63,63	0
56	MG	1H	201	1/1	0.64	0.32	69,69,69,69	0
56	MG	2A	3425	1/1	0.64	0.19	69,69,69,69	0
56	MG	2y	103	1/1	0.64	0.26	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3132	1/1	0.65	0.55	52,52,52,52	0
56	MG	2a	1642	1/1	0.65	0.25	74,74,74,74	0
56	MG	1E	306	1/1	0.65	0.25	59,59,59,59	0
56	MG	2A	3377	1/1	0.65	0.22	70,70,70,70	0
56	MG	2A	3574	1/1	0.65	0.31	66,66,66,66	0
56	MG	1A	3604	1/1	0.65	0.17	27,27,27,27	0
56	MG	2A	3282	1/1	0.65	0.23	68,68,68,68	0
56	MG	1A	3349	1/1	0.65	0.15	65,65,65,65	0
56	MG	1A	3394	1/1	0.65	0.34	78,78,78,78	0
59	ZN	24	501	1/1	0.65	0.06	128,128,128,128	0
56	MG	1A	3467	1/1	0.66	0.21	67,67,67,67	0
56	MG	2A	3781	1/1	0.66	0.56	60,60,60,60	0
56	MG	1A	3993	1/1	0.66	0.10	68,68,68,68	0
56	MG	2A	3508	1/1	0.66	0.39	64,64,64,64	0
56	MG	2A	3390	1/1	0.66	0.21	76,76,76,76	0
56	MG	1A	3634	1/1	0.66	0.14	38,38,38,38	0
56	MG	2A	3395	1/1	0.66	0.17	75,75,75,75	0
56	MG	2A	3119	1/1	0.66	0.47	70,70,70,70	0
56	MG	1A	3207	1/1	0.66	0.12	66,66,66,66	0
56	MG	25	101	1/1	0.66	0.24	64,64,64,64	0
56	MG	2F	301	1/1	0.67	0.22	71,71,71,71	0
56	MG	2A	3269	1/1	0.67	0.14	71,71,71,71	0
56	MG	1A	3549	1/1	0.67	0.23	46,46,46,46	0
56	MG	2a	1708	1/1	0.67	0.27	70,70,70,70	0
56	MG	1a	1735	1/1	0.67	0.15	35,35,35,35	0
56	MG	1a	1739	1/1	0.67	0.33	69,69,69,69	0
56	MG	1A	3928	1/1	0.67	0.14	60,60,60,60	0
56	MG	1A	3672	1/1	0.67	0.14	49,49,49,49	0
56	MG	1A	4008	1/1	0.68	0.26	79,79,79,79	0
56	MG	2A	3639	1/1	0.68	0.39	62,62,62,62	0
56	MG	1A	3834	1/1	0.68	0.17	51,51,51,51	0
56	MG	1A	3412	1/1	0.68	0.36	70,70,70,70	0
56	MG	2A	3392	1/1	0.68	0.20	72,72,72,72	0
56	MG	2A	3345	1/1	0.68	0.18	73,73,73,73	0
56	MG	1a	1740	1/1	0.68	0.24	54,54,54,54	0
56	MG	2A	3369	1/1	0.68	0.16	68,68,68,68	0
56	MG	2A	3031	1/1	0.69	0.36	64,64,64,64	0
56	MG	1A	3523	1/1	0.69	0.10	65,65,65,65	0
56	MG	2a	1633	1/1	0.69	0.27	68,68,68,68	0
56	MG	1A	3888	1/1	0.69	0.13	68,68,68,68	0
56	MG	1A	3911	1/1	0.69	0.45	73,73,73,73	0
56	MG	2A	3817	1/1	0.69	0.15	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	4015	1/1	0.69	0.14	72,72,72,72	0
56	MG	1A	3366	1/1	0.69	0.42	78,78,78,78	0
56	MG	2B	217	1/1	0.69	0.14	58,58,58,58	0
56	MG	2A	3167	1/1	0.69	0.14	80,80,80,80	0
56	MG	1P	202	1/1	0.69	0.52	57,57,57,57	0
56	MG	1A	3801	1/1	0.70	0.23	48,48,48,48	0
56	MG	2A	3624	1/1	0.70	0.16	74,74,74,74	0
56	MG	2A	3436	1/1	0.70	0.16	71,71,71,71	0
56	MG	1A	3945	1/1	0.70	0.15	55,55,55,55	0
56	MG	1A	3095	1/1	0.70	0.24	54,54,54,54	0
56	MG	2A	3152	1/1	0.70	0.17	73,73,73,73	0
56	MG	2A	3776	1/1	0.70	0.28	61,61,61,61	0
56	MG	2a	1825	1/1	0.70	0.22	72,72,72,72	0
56	MG	2i	201	1/1	0.70	0.16	78,78,78,78	0
56	MG	2A	3089	1/1	0.70	0.16	69,69,69,69	0
56	MG	1A	4048	1/1	0.70	0.19	48,48,48,48	0
56	MG	2A	3129	1/1	0.71	0.12	71,71,71,71	0
56	MG	1A	4142	1/1	0.71	0.32	65,65,65,65	0
56	MG	2A	3460	1/1	0.71	0.22	68,68,68,68	0
56	MG	2A	3834	1/1	0.71	0.15	34,34,34,34	0
56	MG	1a	1792	1/1	0.71	0.09	58,58,58,58	0
56	MG	1a	1797	1/1	0.71	0.16	62,62,62,62	0
56	MG	2A	3318	1/1	0.71	0.12	62,62,62,62	0
56	MG	2A	3393	1/1	0.71	0.31	76,76,76,76	0
56	MG	1A	3302	1/1	0.71	0.15	61,61,61,61	0
56	MG	2A	3684	1/1	0.71	0.29	77,77,77,77	0
56	MG	2a	1714	1/1	0.71	0.15	81,81,81,81	0
56	MG	2j	202	1/1	0.71	0.11	79,79,79,79	0
56	MG	2a	1737	1/1	0.71	0.15	84,84,84,84	0
56	MG	2A	3382	1/1	0.71	0.21	67,67,67,67	0
56	MG	2A	3285	1/1	0.72	0.57	64,64,64,64	0
56	MG	2A	3632	1/1	0.72	0.17	68,68,68,68	0
56	MG	1D	303	1/1	0.72	0.26	45,45,45,45	0
56	MG	1A	3489	1/1	0.72	0.97	55,55,55,55	0
56	MG	1A	3236	1/1	0.72	0.31	59,59,59,59	0
56	MG	2a	1611	1/1	0.72	0.24	69,69,69,69	0
56	MG	2A	3319	1/1	0.72	0.38	58,58,58,58	0
56	MG	1A	4016	1/1	0.72	0.16	58,58,58,58	0
56	MG	2a	1812	1/1	0.72	0.15	74,74,74,74	0
56	MG	1a	1607	1/1	0.72	0.11	64,64,64,64	0
56	MG	2A	3699	1/1	0.72	0.20	81,81,81,81	0
56	MG	1A	3760	1/1	0.72	0.24	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	1650	1/1	0.72	0.24	69,69,69,69	0
56	MG	2a	1822	1/1	0.72	0.16	74,74,74,74	0
56	MG	1A	4037	1/1	0.72	0.13	42,42,42,42	0
56	MG	1A	3553	1/1	0.72	0.43	46,46,46,46	0
56	MG	2A	3802	1/1	0.72	0.15	76,76,76,76	0
56	MG	2A	3421	1/1	0.72	0.34	61,61,61,61	0
56	MG	1a	1828	1/1	0.72	0.12	57,57,57,57	0
56	MG	2A	3294	1/1	0.73	0.26	61,61,61,61	0
56	MG	2A	3726	1/1	0.73	0.10	70,70,70,70	0
56	MG	2a	1792	1/1	0.73	0.28	82,82,82,82	0
56	MG	2A	3328	1/1	0.73	0.16	70,70,70,70	0
56	MG	2a	1796	1/1	0.73	0.15	66,66,66,66	0
56	MG	2A	3526	1/1	0.73	0.31	61,61,61,61	0
56	MG	2A	3640	1/1	0.73	0.18	48,48,48,48	0
56	MG	2B	203	1/1	0.73	0.64	62,62,62,62	0
56	MG	2B	210	1/1	0.73	0.16	61,61,61,61	0
56	MG	2A	3329	1/1	0.73	0.30	68,68,68,68	0
56	MG	2A	3808	1/1	0.73	0.12	72,72,72,72	0
56	MG	1A	3689	1/1	0.73	0.15	25,25,25,25	0
56	MG	2a	1721	1/1	0.73	0.35	72,72,72,72	0
56	MG	2a	1736	1/1	0.73	0.04	84,84,84,84	0
56	MG	1A	3222	1/1	0.73	0.36	49,49,49,49	0
56	MG	2x	104	1/1	0.73	0.19	72,72,72,72	0
56	MG	2A	3836	1/1	0.73	0.20	91,91,91,91	0
56	MG	2A	3838	1/1	0.73	0.38	83,83,83,83	0
56	MG	2A	3353	1/1	0.74	0.19	66,66,66,66	0
56	MG	2a	1723	1/1	0.74	0.15	66,66,66,66	0
56	MG	1A	3810	1/1	0.74	0.17	61,61,61,61	0
56	MG	1A	3125	1/1	0.74	0.73	34,34,34,34	0
56	MG	2A	3711	1/1	0.74	0.21	62,62,62,62	0
56	MG	1A	3376	1/1	0.74	0.48	51,51,51,51	0
56	MG	2P	201	1/1	0.74	0.14	63,63,63,63	0
56	MG	2A	3258	1/1	0.74	0.33	61,61,61,61	0
56	MG	2a	1678	1/1	0.74	0.13	57,57,57,57	0
56	MG	2A	3600	1/1	0.74	0.14	37,37,37,37	0
56	MG	1a	1688	1/1	0.74	0.25	63,63,63,63	0
56	MG	1a	1836	1/1	0.74	0.15	64,64,64,64	0
56	MG	1A	3981	1/1	0.75	0.29	51,51,51,51	0
56	MG	1A	3577	1/1	0.75	0.25	46,46,46,46	0
56	MG	2A	3480	1/1	0.75	0.20	66,66,66,66	0
56	MG	1A	3480	1/1	0.75	0.38	44,44,44,44	0
56	MG	1a	1749	1/1	0.75	0.12	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	1770	1/1	0.75	0.16	58,58,58,58	0
56	MG	2a	1780	1/1	0.75	0.18	67,67,67,67	0
56	MG	2a	1641	1/1	0.75	0.27	70,70,70,70	0
56	MG	2A	3256	1/1	0.75	0.20	71,71,71,71	0
56	MG	2A	3120	1/1	0.75	0.24	59,59,59,59	0
56	MG	2A	3524	1/1	0.75	0.27	69,69,69,69	0
56	MG	2A	3266	1/1	0.75	0.23	45,45,45,45	0
56	MG	1A	3469	1/1	0.75	0.19	66,66,66,66	0
56	MG	2a	1670	1/1	0.75	0.12	63,63,63,63	0
56	MG	1w	106	1/1	0.75	0.06	77,77,77,77	0
56	MG	2A	3275	1/1	0.75	0.25	58,58,58,58	0
56	MG	10	103	1/1	0.75	0.35	42,42,42,42	0
56	MG	1A	3978	1/1	0.75	0.44	78,78,78,78	0
56	MG	1A	3940	1/1	0.75	0.10	76,76,76,76	0
56	MG	1a	1645	1/1	0.75	0.12	59,59,59,59	0
56	MG	2A	3367	1/1	0.75	0.39	65,65,65,65	0
56	MG	2a	1733	1/1	0.75	0.35	96,96,96,96	0
56	MG	2W	202	1/1	0.75	0.78	66,66,66,66	0
56	MG	1A	3498	1/1	0.76	1.10	61,61,61,61	0
56	MG	1y	103	1/1	0.76	0.34	76,76,76,76	0
56	MG	2A	3404	1/1	0.76	0.89	58,58,58,58	0
56	MG	2A	3182	1/1	0.76	0.12	37,37,37,37	0
56	MG	2B	209	1/1	0.76	0.13	66,66,66,66	0
56	MG	2A	3214	1/1	0.76	0.30	49,49,49,49	0
56	MG	2A	3228	1/1	0.76	0.31	68,68,68,68	0
56	MG	2A	3675	1/1	0.76	0.15	55,55,55,55	0
56	MG	10	105	1/1	0.76	0.14	50,50,50,50	0
56	MG	2Q	201	1/1	0.76	0.13	72,72,72,72	0
56	MG	1A	3972	1/1	0.76	0.16	20,20,20,20	0
56	MG	2A	3452	1/1	0.76	0.15	67,67,67,67	0
56	MG	1A	3080	1/1	0.76	0.17	55,55,55,55	0
56	MG	1a	1686	1/1	0.76	0.37	62,62,62,62	0
56	MG	1A	3456	1/1	0.76	0.17	56,56,56,56	0
56	MG	2a	1627	1/1	0.76	0.45	63,63,63,63	0
56	MG	2A	3362	1/1	0.76	0.36	69,69,69,69	0
56	MG	1a	1717	1/1	0.76	0.18	48,48,48,48	0
56	MG	1A	3289	1/1	0.76	0.12	46,46,46,46	0
56	MG	1A	3224	1/1	0.76	0.76	46,46,46,46	0
56	MG	2A	3280	1/1	0.76	0.27	59,59,59,59	0
56	MG	1A	4086	1/1	0.76	0.17	62,62,62,62	0
56	MG	1A	3790	1/1	0.76	0.12	52,52,52,52	0
56	MG	2f	202	1/1	0.76	0.15	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	1a	1794	1/1	0.76	0.40	83,83,83,83	0
56	MG	2A	3570	1/1	0.76	0.12	32,32,32,32	0
56	MG	1A	4035	1/1	0.76	0.18	31,31,31,31	0
56	MG	1A	4146	1/1	0.76	0.81	45,45,45,45	0
56	MG	2A	3164	1/1	0.76	0.14	66,66,66,66	0
56	MG	2A	3317	1/1	0.77	0.83	74,74,74,74	0
56	MG	2a	1719	1/1	0.77	0.47	75,75,75,75	0
56	MG	1A	3133	1/1	0.77	0.52	46,46,46,46	0
56	MG	1A	3668	1/1	0.77	0.16	28,28,28,28	0
56	MG	1A	3345	1/1	0.77	0.24	56,56,56,56	0
56	MG	2A	3731	1/1	0.77	0.19	45,45,45,45	0
56	MG	2A	3756	1/1	0.77	0.15	71,71,71,71	0
56	MG	2A	3765	1/1	0.77	0.26	54,54,54,54	0
56	MG	1A	3587	1/1	0.77	0.23	51,51,51,51	0
56	MG	2A	3394	1/1	0.77	0.29	78,78,78,78	0
56	MG	2A	3030	1/1	0.77	0.26	68,68,68,68	0
56	MG	2a	1763	1/1	0.77	0.22	85,85,85,85	0
56	MG	2A	3795	1/1	0.77	0.14	51,51,51,51	0
56	MG	2A	3396	1/1	0.77	0.21	62,62,62,62	0
56	MG	2A	3402	1/1	0.77	0.35	76,76,76,76	0
56	MG	1a	1742	1/1	0.77	0.18	77,77,77,77	0
56	MG	1A	3949	1/1	0.77	0.13	29,29,29,29	0
56	MG	2a	1637	1/1	0.77	0.34	68,68,68,68	0
56	MG	1a	1777	1/1	0.77	0.09	59,59,59,59	0
56	MG	1a	1789	1/1	0.77	0.28	47,47,47,47	0
56	MG	1A	3518	1/1	0.77	0.91	53,53,53,53	0
56	MG	1A	3969	1/1	0.77	0.16	20,20,20,20	0
56	MG	2A	3358	1/1	0.77	0.16	53,53,53,53	0
56	MG	2a	1653	1/1	0.77	0.34	87,87,87,87	0
56	MG	1A	3084	1/1	0.77	0.15	38,38,38,38	0
56	MG	1A	3625	1/1	0.77	0.09	39,39,39,39	0
56	MG	2A	3309	1/1	0.77	0.16	75,75,75,75	0
56	MG	1G	203	1/1	0.77	0.38	64,64,64,64	0
56	MG	2A	3312	1/1	0.77	0.53	71,71,71,71	0
56	MG	2a	1706	1/1	0.77	0.28	65,65,65,65	0
56	MG	2y	107	1/1	0.77	0.09	95,95,95,95	0
56	MG	1y	104	1/1	0.77	0.38	87,87,87,87	0
56	MG	1A	3340	1/1	0.78	0.17	59,59,59,59	0
56	MG	2a	1691	1/1	0.78	0.12	74,74,74,74	0
56	MG	1A	3958	1/1	0.78	0.12	73,73,73,73	0
56	MG	2A	3815	1/1	0.78	0.28	80,80,80,80	0
56	MG	1A	3960	1/1	0.78	0.15	38,38,38,38	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	0.78	0.08	44,44,44,44	0
56	MG	1A	3436	1/1	0.78	0.91	38,38,38,38	0
56	MG	1b	301	1/1	0.78	0.09	82,82,82,82	0
56	MG	1A	3905	1/1	0.78	0.19	55,55,55,55	0
56	MG	1A	3906	1/1	0.78	0.40	58,58,58,58	0
56	MG	1A	3002	1/1	0.78	0.28	57,57,57,57	0
56	MG	1A	3563	1/1	0.78	0.24	47,47,47,47	0
56	MG	2A	3630	1/1	0.78	0.21	73,73,73,73	0
56	MG	1A	3792	1/1	0.78	0.10	29,29,29,29	0
56	MG	2a	1746	1/1	0.78	0.11	51,51,51,51	0
56	MG	2a	1752	1/1	0.78	0.07	76,76,76,76	0
56	MG	2A	3166	1/1	0.78	0.10	67,67,67,67	0
56	MG	2A	3320	1/1	0.78	0.13	75,75,75,75	0
56	MG	1A	3463	1/1	0.78	0.93	53,53,53,53	0
56	MG	1A	3650	1/1	0.78	0.17	36,36,36,36	0
56	MG	1A	3821	1/1	0.78	0.21	64,64,64,64	0
56	MG	1A	4005	1/1	0.78	0.10	53,53,53,53	0
56	MG	1a	1667	1/1	0.78	0.10	73,73,73,73	0
56	MG	1A	4147	1/1	0.78	0.16	27,27,27,27	0
56	MG	2a	1800	1/1	0.78	0.20	71,71,71,71	0
56	MG	2A	3451	1/1	0.78	0.24	61,61,61,61	0
56	MG	2A	3348	1/1	0.78	0.25	62,62,62,62	0
56	MG	1a	1693	1/1	0.78	0.15	62,62,62,62	0
56	MG	2A	3457	1/1	0.78	0.38	66,66,66,66	0
56	MG	2A	3734	1/1	0.78	0.46	51,51,51,51	0
56	MG	2A	3352	1/1	0.78	0.64	66,66,66,66	0
56	MG	2A	3019	1/1	0.78	0.21	65,65,65,65	0
56	MG	1A	3943	1/1	0.78	0.09	58,58,58,58	0
56	MG	2a	1829	1/1	0.78	0.12	69,69,69,69	0
56	MG	2A	3496	1/1	0.78	0.19	50,50,50,50	0
56	MG	1a	1764	1/1	0.78	0.14	58,58,58,58	0
56	MG	1a	1767	1/1	0.78	0.08	91,91,91,91	0
56	MG	2w	101	1/1	0.78	0.14	70,70,70,70	0
56	MG	2A	3500	1/1	0.78	0.12	49,49,49,49	0
56	MG	1a	1781	1/1	0.78	0.14	66,66,66,66	0
56	MG	1A	3361	1/1	0.78	0.39	57,57,57,57	0
56	MG	2a	1676	1/1	0.78	0.29	66,66,66,66	0
56	MG	2A	3308	1/1	0.79	0.64	69,69,69,69	0
56	MG	1A	3260	1/1	0.79	0.25	44,44,44,44	0
56	MG	1B	223	1/1	0.79	0.21	57,57,57,57	0
56	MG	2A	3397	1/1	0.79	0.17	67,67,67,67	0
56	MG	2A	3130	1/1	0.79	0.27	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	2a	1758	1/1	0.79	0.07	64,64,64,64	0
56	MG	2A	3688	1/1	0.79	0.16	53,53,53,53	0
56	MG	1A	3381	1/1	0.79	0.23	52,52,52,52	0
56	MG	2a	1647	1/1	0.79	0.58	56,56,56,56	0
56	MG	1A	3998	1/1	0.79	0.12	24,24,24,24	0
56	MG	1A	3920	1/1	0.79	0.09	41,41,41,41	0
56	MG	1U	202	1/1	0.79	0.79	56,56,56,56	0
56	MG	1Y	202	1/1	0.79	0.17	65,65,65,65	0
56	MG	2A	3058	1/1	0.79	0.15	54,54,54,54	0
56	MG	2a	1662	1/1	0.79	0.22	51,51,51,51	0
56	MG	2A	3435	1/1	0.79	0.29	54,54,54,54	0
56	MG	2A	3735	1/1	0.79	0.20	68,68,68,68	0
56	MG	2A	3278	1/1	0.79	0.19	54,54,54,54	0
56	MG	2A	3582	1/1	0.79	0.15	39,39,39,39	0
56	MG	2a	1685	1/1	0.79	0.20	60,60,60,60	0
56	MG	1A	3354	1/1	0.79	0.15	59,59,59,59	0
56	MG	2a	1824	1/1	0.79	0.21	71,71,71,71	0
56	MG	1A	4043	1/1	0.79	0.08	44,44,44,44	0
56	MG	2A	3615	1/1	0.79	0.09	57,57,57,57	0
56	MG	2A	3790	1/1	0.79	0.17	82,82,82,82	0
56	MG	2A	3456	1/1	0.79	0.18	70,70,70,70	0
56	MG	1A	3843	1/1	0.79	0.17	65,65,65,65	0
56	MG	1a	1721	1/1	0.79	0.11	54,54,54,54	0
56	MG	2A	3196	1/1	0.79	0.14	40,40,40,40	0
56	MG	2A	3463	1/1	0.79	0.22	54,54,54,54	0
56	MG	1A	3737	1/1	0.79	0.16	66,66,66,66	0
56	MG	2A	3653	1/1	0.79	0.28	60,60,60,60	0
56	MG	2A	3442	1/1	0.80	0.31	59,59,59,59	0
56	MG	1A	3287	1/1	0.80	0.18	54,54,54,54	0
56	MG	1A	3217	1/1	0.80	0.90	46,46,46,46	0
56	MG	1A	3639	1/1	0.80	0.17	70,70,70,70	0
56	MG	1A	3026	1/1	0.80	0.73	43,43,43,43	0
56	MG	1A	3665	1/1	0.80	0.19	22,22,22,22	0
56	MG	1A	3178	1/1	0.80	1.22	47,47,47,47	0
56	MG	2a	1727	1/1	0.80	0.14	63,63,63,63	0
56	MG	12	101	1/1	0.80	0.40	56,56,56,56	0
56	MG	2A	3477	1/1	0.80	0.27	56,56,56,56	0
56	MG	2B	214	1/1	0.80	0.19	71,71,71,71	0
56	MG	2a	1739	1/1	0.80	0.13	76,76,76,76	0
56	MG	2a	1740	1/1	0.80	0.14	69,69,69,69	0
56	MG	1A	3397	1/1	0.80	0.47	33,33,33,33	0
56	MG	1a	1638	1/1	0.80	0.22	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	3730	1/1	0.80	0.14	32,32,32,32	0
56	MG	1a	1660	1/1	0.80	0.52	43,43,43,43	0
56	MG	2a	1755	1/1	0.80	0.13	78,78,78,78	0
56	MG	1A	3404	1/1	0.80	0.17	53,53,53,53	0
56	MG	2A	3009	1/1	0.80	0.24	60,60,60,60	0
56	MG	25	104	1/1	0.80	0.36	65,65,65,65	0
56	MG	1A	3406	1/1	0.80	0.16	54,54,54,54	0
56	MG	2A	3027	1/1	0.80	0.24	45,45,45,45	0
56	MG	1A	3359	1/1	0.80	0.25	50,50,50,50	0
56	MG	1a	1706	1/1	0.80	0.12	59,59,59,59	0
56	MG	1A	3413	1/1	0.80	0.10	56,56,56,56	0
56	MG	2A	3054	1/1	0.80	0.11	82,82,82,82	0
56	MG	1A	4041	1/1	0.80	0.14	25,25,25,25	0
56	MG	1A	3425	1/1	0.80	1.10	57,57,57,57	0
56	MG	1A	3600	1/1	0.80	0.13	42,42,42,42	0
56	MG	2A	3405	1/1	0.80	0.73	68,68,68,68	0
56	MG	2A	3586	1/1	0.80	0.13	32,32,32,32	0
56	MG	2a	1651	1/1	0.80	0.13	85,85,85,85	0
56	MG	2A	3597	1/1	0.80	0.12	66,66,66,66	0
56	MG	2A	3108	1/1	0.80	0.15	61,61,61,61	0
56	MG	2A	3272	1/1	0.80	0.20	64,64,64,64	0
56	MG	2a	1661	1/1	0.80	0.17	83,83,83,83	0
56	MG	2A	3422	1/1	0.80	0.17	63,63,63,63	0
56	MG	2A	3350	1/1	0.80	0.13	63,63,63,63	0
56	MG	2A	3840	1/1	0.80	0.10	72,72,72,72	0
56	MG	2A	3426	1/1	0.80	0.69	63,63,63,63	0
56	MG	2A	3351	1/1	0.80	0.27	64,64,64,64	0
56	MG	2a	1682	1/1	0.80	0.11	68,68,68,68	0
56	MG	1A	3017	1/1	0.80	0.42	55,55,55,55	0
56	MG	2A	3441	1/1	0.80	0.59	56,56,56,56	0
56	MG	2a	1692	1/1	0.80	0.13	65,65,65,65	0
56	MG	1A	3595	1/1	0.81	0.60	46,46,46,46	0
56	MG	2A	3604	1/1	0.81	0.10	52,52,52,52	0
56	MG	2A	3605	1/1	0.81	0.22	62,62,62,62	0
56	MG	2B	212	1/1	0.81	0.15	69,69,69,69	0
56	MG	1A	3185	1/1	0.81	0.50	39,39,39,39	0
56	MG	1a	1687	1/1	0.81	0.52	57,57,57,57	0
56	MG	2B	218	1/1	0.81	0.13	76,76,76,76	0
56	MG	1A	3950	1/1	0.81	0.12	62,62,62,62	0
56	MG	2O	201	1/1	0.81	0.09	64,64,64,64	0
56	MG	2A	3386	1/1	0.81	0.16	61,61,61,61	0
56	MG	2A	3227	1/1	0.81	0.28	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3956	1/1	0.81	0.28	49,49,49,49	0
56	MG	2A	3253	1/1	0.81	0.16	38,38,38,38	0
56	MG	2A	3323	1/1	0.81	0.30	54,54,54,54	0
56	MG	2A	3473	1/1	0.81	0.29	54,54,54,54	0
56	MG	2a	1615	1/1	0.81	0.15	60,60,60,60	0
56	MG	1A	3537	1/1	0.81	0.20	56,56,56,56	0
56	MG	2a	1757	1/1	0.81	0.14	76,76,76,76	0
56	MG	1A	3418	1/1	0.81	0.43	42,42,42,42	0
56	MG	1A	3913	1/1	0.81	0.08	70,70,70,70	0
56	MG	2a	1630	1/1	0.81	0.43	71,71,71,71	0
56	MG	1A	3257	1/1	0.81	0.12	62,62,62,62	0
56	MG	1a	1753	1/1	0.81	0.11	47,47,47,47	0
56	MG	2A	3344	1/1	0.81	0.16	67,67,67,67	0
56	MG	1A	3228	1/1	0.81	0.62	25,25,25,25	0
56	MG	1A	4148	1/1	0.81	0.56	59,59,59,59	0
56	MG	1N	203	1/1	0.81	0.43	41,41,41,41	0
56	MG	1a	1786	1/1	0.81	0.11	53,53,53,53	0
56	MG	2a	1808	1/1	0.81	0.26	75,75,75,75	0
56	MG	1N	207	1/1	0.81	0.49	59,59,59,59	0
56	MG	2a	1814	1/1	0.81	0.18	59,59,59,59	0
56	MG	2A	3409	1/1	0.81	0.20	67,67,67,67	0
56	MG	1A	3492	1/1	0.81	0.29	40,40,40,40	0
56	MG	1a	1795	1/1	0.81	0.11	71,71,71,71	0
56	MG	1A	3364	1/1	0.81	0.78	55,55,55,55	0
56	MG	1a	1806	1/1	0.81	0.11	67,67,67,67	0
56	MG	2a	1668	1/1	0.81	0.12	55,55,55,55	0
56	MG	1a	1812	1/1	0.81	0.13	55,55,55,55	0
56	MG	1a	1814	1/1	0.81	0.20	84,84,84,84	0
56	MG	1A	3308	1/1	0.81	0.15	64,64,64,64	0
56	MG	1A	3367	1/1	0.81	0.42	51,51,51,51	0
56	MG	2j	201	1/1	0.81	0.15	58,58,58,58	0
56	MG	2A	3755	1/1	0.81	0.12	54,54,54,54	0
56	MG	1A	3368	1/1	0.81	0.26	53,53,53,53	0
56	MG	17	101	1/1	0.81	0.36	34,34,34,34	0
56	MG	1a	1605	1/1	0.81	0.13	56,56,56,56	0
56	MG	2A	3040	1/1	0.81	0.11	68,68,68,68	0
56	MG	2A	3180	1/1	0.81	0.20	42,42,42,42	0
56	MG	1a	1755	1/1	0.82	0.06	51,51,51,51	0
56	MG	1a	1757	1/1	0.82	0.12	56,56,56,56	0
56	MG	2A	3437	1/1	0.82	0.39	66,66,66,66	0
56	MG	1a	1766	1/1	0.82	0.15	53,53,53,53	0
56	MG	2A	3219	1/1	0.82	0.15	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	1773	1/1	0.82	0.14	56,56,56,56	0
56	MG	2A	3379	1/1	0.82	0.13	58,58,58,58	0
56	MG	2A	3445	1/1	0.82	0.19	67,67,67,67	0
56	MG	2A	3225	1/1	0.82	0.21	63,63,63,63	0
56	MG	1A	3162	1/1	0.82	0.15	63,63,63,63	0
56	MG	2A	3845	1/1	0.82	0.55	66,66,66,66	0
56	MG	1B	204	1/1	0.82	0.16	52,52,52,52	0
56	MG	1B	220	1/1	0.82	0.17	65,65,65,65	0
56	MG	2a	1707	1/1	0.82	1.27	76,76,76,76	0
56	MG	2A	3453	1/1	0.82	0.28	77,77,77,77	0
56	MG	1B	225	1/1	0.82	0.09	56,56,56,56	0
56	MG	1A	3872	1/1	0.82	0.13	64,64,64,64	0
56	MG	2A	3239	1/1	0.82	0.12	52,52,52,52	0
56	MG	2A	3643	1/1	0.82	0.15	29,29,29,29	0
56	MG	1A	3770	1/1	0.82	0.12	39,39,39,39	0
56	MG	2A	3461	1/1	0.82	0.20	65,65,65,65	0
56	MG	1A	3270	1/1	0.82	0.10	39,39,39,39	0
56	MG	2A	3465	1/1	0.82	0.22	33,33,33,33	0
56	MG	1y	102	1/1	0.82	0.21	63,63,63,63	0
56	MG	1A	3194	1/1	0.82	0.18	55,55,55,55	0
56	MG	2A	3686	1/1	0.82	0.12	64,64,64,64	0
56	MG	2B	201	1/1	0.82	0.22	81,81,81,81	0
56	MG	2A	3260	1/1	0.82	0.20	51,51,51,51	0
56	MG	1Z	303	1/1	0.82	0.17	54,54,54,54	0
56	MG	2A	3695	1/1	0.82	0.10	52,52,52,52	0
56	MG	10	104	1/1	0.82	0.69	41,41,41,41	0
56	MG	1A	3083	1/1	0.82	0.82	52,52,52,52	0
56	MG	10	107	1/1	0.82	0.37	67,67,67,67	0
56	MG	2a	1760	1/1	0.82	0.09	81,81,81,81	0
56	MG	2A	3701	1/1	0.82	0.11	54,54,54,54	0
56	MG	1A	3216	1/1	0.82	0.19	46,46,46,46	0
56	MG	2A	3151	1/1	0.82	0.62	51,51,51,51	0
56	MG	2A	3039	1/1	0.82	0.19	88,88,88,88	0
56	MG	1A	3959	1/1	0.82	0.17	69,69,69,69	0
56	MG	1a	1637	1/1	0.82	0.09	60,60,60,60	0
56	MG	2A	3053	1/1	0.82	0.19	69,69,69,69	0
56	MG	1A	3705	1/1	0.82	0.10	70,70,70,70	0
56	MG	2A	3740	1/1	0.82	0.15	50,50,50,50	0
56	MG	2a	1606	1/1	0.82	0.19	61,61,61,61	0
56	MG	1a	1661	1/1	0.82	0.10	72,72,72,72	0
56	MG	2A	3746	1/1	0.82	0.16	65,65,65,65	0
56	MG	2a	1616	1/1	0.82	0.33	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	1620	1/1	0.82	0.50	80,80,80,80	0
56	MG	1a	1668	1/1	0.82	0.21	68,68,68,68	0
56	MG	2A	3753	1/1	0.82	0.09	50,50,50,50	0
56	MG	2A	3419	1/1	0.82	0.49	69,69,69,69	0
56	MG	2A	3529	1/1	0.82	0.11	67,67,67,67	0
56	MG	2A	3764	1/1	0.82	0.22	60,60,60,60	0
56	MG	1A	3717	1/1	0.82	0.19	74,74,74,74	0
56	MG	2A	3561	1/1	0.82	0.20	64,64,64,64	0
56	MG	2A	3355	1/1	0.82	0.34	67,67,67,67	0
56	MG	1A	3736	1/1	0.82	0.23	76,76,76,76	0
56	MG	2A	3788	1/1	0.82	0.13	64,64,64,64	0
56	MG	2l	202	1/1	0.82	0.13	60,60,60,60	0
56	MG	2v	102	1/1	0.82	0.46	79,79,79,79	0
56	MG	2A	3193	1/1	0.82	0.45	53,53,53,53	0
56	MG	2A	3431	1/1	0.82	0.24	52,52,52,52	0
56	MG	1A	3290	1/1	0.82	0.13	49,49,49,49	0
56	MG	1A	3862	1/1	0.82	0.79	44,44,44,44	0
56	MG	2A	3814	1/1	0.82	0.21	64,64,64,64	0
56	MG	1A	3256	1/1	0.83	0.20	64,64,64,64	0
56	MG	1A	3852	1/1	0.83	0.14	54,54,54,54	0
56	MG	2A	3267	1/1	0.83	0.54	64,64,64,64	0
56	MG	2A	3820	1/1	0.83	0.07	49,49,49,49	0
56	MG	2A	3822	1/1	0.83	0.31	63,63,63,63	0
56	MG	2A	3829	1/1	0.83	0.16	61,61,61,61	0
56	MG	2A	3486	1/1	0.83	0.25	53,53,53,53	0
56	MG	1A	3230	1/1	0.83	0.30	50,50,50,50	0
56	MG	1A	3526	1/1	0.83	0.27	50,50,50,50	0
56	MG	2A	3502	1/1	0.83	0.11	52,52,52,52	0
56	MG	1A	3365	1/1	0.83	0.20	38,38,38,38	0
56	MG	2A	3507	1/1	0.83	0.12	50,50,50,50	0
56	MG	1A	3883	1/1	0.83	0.16	31,31,31,31	0
56	MG	2R	202	1/1	0.83	0.26	59,59,59,59	0
56	MG	2A	3519	1/1	0.83	0.21	50,50,50,50	0
56	MG	1A	3885	1/1	0.83	0.25	61,61,61,61	0
56	MG	1a	1741	1/1	0.83	0.08	48,48,48,48	0
56	MG	1A	4028	1/1	0.83	0.12	31,31,31,31	0
56	MG	1A	3348	1/1	0.83	0.12	54,54,54,54	0
56	MG	2A	3534	1/1	0.83	0.11	45,45,45,45	0
56	MG	1A	3607	1/1	0.83	0.15	61,61,61,61	0
56	MG	1A	3544	1/1	0.83	0.63	49,49,49,49	0
56	MG	2A	3304	1/1	0.83	0.19	66,66,66,66	0
56	MG	2a	1769	1/1	0.83	0.10	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3376	1/1	0.83	0.77	73,73,73,73	0
56	MG	1O	201	1/1	0.83	0.47	60,60,60,60	0
56	MG	2A	3052	1/1	0.83	0.10	60,60,60,60	0
56	MG	1a	1775	1/1	0.83	0.14	59,59,59,59	0
56	MG	1A	3283	1/1	0.83	0.52	55,55,55,55	0
56	MG	1A	3167	1/1	0.83	0.14	36,36,36,36	0
56	MG	2a	1802	1/1	0.83	0.26	75,75,75,75	0
56	MG	1A	3372	1/1	0.83	0.29	51,51,51,51	0
56	MG	2A	3387	1/1	0.83	0.17	61,61,61,61	0
56	MG	1a	1790	1/1	0.83	0.13	54,54,54,54	0
56	MG	1A	3803	1/1	0.83	0.22	60,60,60,60	0
56	MG	2A	3071	1/1	0.83	0.16	61,61,61,61	0
56	MG	1A	3656	1/1	0.83	0.14	23,23,23,23	0
56	MG	2A	3784	1/1	0.83	0.11	47,47,47,47	0
56	MG	1A	3357	1/1	0.83	0.14	72,72,72,72	0
56	MG	2A	3327	1/1	0.83	0.17	67,67,67,67	0
56	MG	2a	1823	1/1	0.83	0.16	61,61,61,61	0
56	MG	1A	3254	1/1	0.83	0.23	47,47,47,47	0
56	MG	2a	1663	1/1	0.83	0.10	77,77,77,77	0
56	MG	1A	3389	1/1	0.83	1.37	45,45,45,45	0
56	MG	1a	1616	1/1	0.83	0.30	55,55,55,55	0
56	MG	1a	1626	1/1	0.83	0.14	44,44,44,44	0
56	MG	1a	1629	1/1	0.83	0.13	59,59,59,59	0
56	MG	1b	302	1/1	0.83	0.07	86,86,86,86	0
56	MG	2A	3805	1/1	0.83	0.12	54,54,54,54	0
56	MG	1x	105	1/1	0.83	0.10	65,65,65,65	0
56	MG	1x	108	1/1	0.83	0.17	73,73,73,73	0
56	MG	1A	4127	1/1	0.83	0.16	40,40,40,40	0
56	MG	2A	3811	1/1	0.83	0.09	45,45,45,45	0
56	MG	2y	105	1/1	0.83	0.28	93,93,93,93	0
56	MG	2a	1703	1/1	0.83	0.30	81,81,81,81	0
56	MG	1a	1658	1/1	0.83	0.17	61,61,61,61	0
56	MG	1A	3531	1/1	0.84	0.25	61,61,61,61	0
56	MG	1w	101	1/1	0.84	0.13	67,67,67,67	0
56	MG	2A	3620	1/1	0.84	0.10	56,56,56,56	0
56	MG	2A	3799	1/1	0.84	0.15	63,63,63,63	0
56	MG	2A	3252	1/1	0.84	0.94	71,71,71,71	0
56	MG	1A	3533	1/1	0.84	0.16	28,28,28,28	0
56	MG	2A	3121	1/1	0.84	0.12	54,54,54,54	0
56	MG	1A	3495	1/1	0.84	0.22	52,52,52,52	0
56	MG	2A	3123	1/1	0.84	0.15	48,48,48,48	0
56	MG	1A	3880	1/1	0.84	0.19	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	4013	1/1	0.84	0.12	65,65,65,65	0
56	MG	2A	3494	1/1	0.84	0.09	66,66,66,66	0
56	MG	1A	3459	1/1	0.84	0.14	62,62,62,62	0
56	MG	2A	3498	1/1	0.84	0.35	59,59,59,59	0
56	MG	2A	3499	1/1	0.84	0.13	50,50,50,50	0
56	MG	1A	3545	1/1	0.84	0.47	53,53,53,53	0
56	MG	2A	3413	1/1	0.84	0.12	55,55,55,55	0
56	MG	2A	3839	1/1	0.84	0.13	64,64,64,64	0
56	MG	2A	3694	1/1	0.84	0.15	44,44,44,44	0
56	MG	1A	3482	1/1	0.84	0.13	51,51,51,51	0
56	MG	1A	3505	1/1	0.84	0.16	75,75,75,75	0
56	MG	1B	210	1/1	0.84	0.22	48,48,48,48	0
56	MG	1B	214	1/1	0.84	0.10	50,50,50,50	0
56	MG	1A	3488	1/1	0.84	0.64	43,43,43,43	0
56	MG	2A	3514	1/1	0.84	0.17	58,58,58,58	0
56	MG	1A	3966	1/1	0.84	0.45	67,67,67,67	0
56	MG	1B	229	1/1	0.84	0.11	62,62,62,62	0
56	MG	1a	1750	1/1	0.84	0.12	53,53,53,53	0
56	MG	2A	3522	1/1	0.84	0.20	62,62,62,62	0
56	MG	2A	3357	1/1	0.84	0.12	59,59,59,59	0
56	MG	1A	3641	1/1	0.84	0.13	32,32,32,32	0
56	MG	1F	308	1/1	0.84	0.18	45,45,45,45	0
56	MG	1F	309	1/1	0.84	0.20	48,48,48,48	0
56	MG	2A	3291	1/1	0.84	0.75	47,47,47,47	0
56	MG	2A	3292	1/1	0.84	0.88	47,47,47,47	0
56	MG	2a	1807	1/1	0.84	0.12	64,64,64,64	0
56	MG	1a	1774	1/1	0.84	0.17	67,67,67,67	0
56	MG	2a	1811	1/1	0.84	0.08	72,72,72,72	0
56	MG	2A	3745	1/1	0.84	0.20	65,65,65,65	0
56	MG	1A	3522	1/1	0.84	0.66	43,43,43,43	0
56	MG	2A	3750	1/1	0.84	0.09	64,64,64,64	0
56	MG	1P	201	1/1	0.84	0.12	36,36,36,36	0
56	MG	1a	1787	1/1	0.84	0.09	64,64,64,64	0
56	MG	1A	3565	1/1	0.84	0.85	46,46,46,46	0
56	MG	1A	3362	1/1	0.84	0.81	47,47,47,47	0
56	MG	1A	3225	1/1	0.84	0.19	45,45,45,45	0
56	MG	2A	3758	1/1	0.84	0.09	66,66,66,66	0
56	MG	2a	1660	1/1	0.84	0.20	66,66,66,66	0
56	MG	1A	3494	1/1	0.84	0.21	58,58,58,58	0
56	MG	1A	3937	1/1	0.84	0.11	55,55,55,55	0
56	MG	1A	3682	1/1	0.84	0.16	33,33,33,33	0
56	MG	2A	3095	1/1	0.84	0.16	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1a	1813	1/1	0.84	0.14	63,63,63,63	0
56	MG	1A	3592	1/1	0.84	0.50	34,34,34,34	0
56	MG	2q	201	1/1	0.84	0.09	63,63,63,63	0
56	MG	1a	1816	1/1	0.84	0.15	52,52,52,52	0
56	MG	1a	1823	1/1	0.84	0.12	43,43,43,43	0
56	MG	2A	3459	1/1	0.84	0.36	62,62,62,62	0
56	MG	15	104	1/1	0.84	0.66	42,42,42,42	0
56	MG	2A	3235	1/1	0.84	0.20	79,79,79,79	0
56	MG	2A	3789	1/1	0.84	0.10	43,43,43,43	0
56	MG	2a	1696	1/1	0.84	0.13	73,73,73,73	0
56	MG	1A	3765	1/1	0.85	0.13	58,58,58,58	0
56	MG	1A	3540	1/1	0.85	0.13	53,53,53,53	0
56	MG	2A	3635	1/1	0.85	0.15	56,56,56,56	0
56	MG	1B	203	1/1	0.85	0.18	48,48,48,48	0
56	MG	2A	3004	1/1	0.85	0.23	82,82,82,82	0
56	MG	2A	3215	1/1	0.85	0.27	60,60,60,60	0
56	MG	1A	3990	1/1	0.85	0.29	65,65,65,65	0
56	MG	1A	3542	1/1	0.85	0.15	49,49,49,49	0
56	MG	2A	3656	1/1	0.85	0.13	33,33,33,33	0
56	MG	1A	3358	1/1	0.85	0.50	62,62,62,62	0
56	MG	1a	1782	1/1	0.85	0.13	59,59,59,59	0
56	MG	1A	3799	1/1	0.85	0.09	52,52,52,52	0
56	MG	1B	230	1/1	0.85	0.18	83,83,83,83	0
56	MG	1A	3055	1/1	0.85	0.18	33,33,33,33	0
56	MG	1A	3927	1/1	0.85	0.08	37,37,37,37	0
56	MG	2A	3241	1/1	0.85	0.25	61,61,61,61	0
56	MG	1A	3030	1/1	0.85	0.12	34,34,34,34	0
56	MG	2A	3691	1/1	0.85	0.28	79,79,79,79	0
56	MG	1A	4011	1/1	0.85	0.27	58,58,58,58	0
56	MG	1A	3804	1/1	0.85	0.37	40,40,40,40	0
56	MG	1a	1808	1/1	0.85	0.20	61,61,61,61	0
56	MG	2A	3366	1/1	0.85	0.47	59,59,59,59	0
56	MG	1A	3417	1/1	0.85	0.19	58,58,58,58	0
56	MG	2a	1718	1/1	0.85	0.17	72,72,72,72	0
56	MG	1A	3054	1/1	0.85	0.12	61,61,61,61	0
56	MG	1A	3822	1/1	0.85	0.37	77,77,77,77	0
56	MG	2A	3487	1/1	0.85	0.16	49,49,49,49	0
56	MG	1A	4020	1/1	0.85	0.60	78,78,78,78	0
56	MG	1A	3827	1/1	0.85	0.17	48,48,48,48	0
56	MG	1a	1834	1/1	0.85	0.12	73,73,73,73	0
56	MG	1Z	302	1/1	0.85	0.38	52,52,52,52	0
56	MG	2A	3271	1/1	0.85	0.13	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	2A	3739	1/1	0.85	0.09	68,68,68,68	0
56	MG	1v	101	1/1	0.85	0.18	67,67,67,67	0
56	MG	1A	4031	1/1	0.85	0.09	38,38,38,38	0
56	MG	2A	3742	1/1	0.85	0.10	58,58,58,58	0
56	MG	2A	3105	1/1	0.85	0.49	57,57,57,57	0
56	MG	1A	3511	1/1	0.85	0.49	67,67,67,67	0
56	MG	2A	3279	1/1	0.85	0.23	54,54,54,54	0
56	MG	2A	3505	1/1	0.85	0.22	54,54,54,54	0
56	MG	1A	3840	1/1	0.85	0.15	22,22,22,22	0
56	MG	1y	105	1/1	0.85	0.13	63,63,63,63	0
56	MG	2a	1761	1/1	0.85	0.08	61,61,61,61	0
56	MG	1A	3419	1/1	0.85	0.29	61,61,61,61	0
56	MG	1A	3957	1/1	0.85	0.24	61,61,61,61	0
56	MG	1A	3424	1/1	0.85	0.89	53,53,53,53	0
56	MG	1A	3678	1/1	0.85	0.11	64,64,64,64	0
56	MG	1A	3679	1/1	0.85	0.12	34,34,34,34	0
56	MG	1a	1634	1/1	0.85	0.28	54,54,54,54	0
56	MG	1a	1636	1/1	0.85	0.25	51,51,51,51	0
56	MG	2a	1794	1/1	0.85	0.11	74,74,74,74	0
56	MG	2A	3296	1/1	0.85	0.68	50,50,50,50	0
56	MG	1A	3478	1/1	0.85	0.47	57,57,57,57	0
56	MG	2a	1801	1/1	0.85	0.12	65,65,65,65	0
56	MG	1A	4063	1/1	0.85	0.15	54,54,54,54	0
56	MG	2F	302	1/1	0.85	0.79	59,59,59,59	0
56	MG	1a	1657	1/1	0.85	0.14	69,69,69,69	0
56	MG	2A	3787	1/1	0.85	0.06	55,55,55,55	0
56	MG	2A	3406	1/1	0.85	0.40	63,63,63,63	0
56	MG	2Q	203	1/1	0.85	0.56	61,61,61,61	0
56	MG	2A	3305	1/1	0.85	0.16	68,68,68,68	0
56	MG	2V	201	1/1	0.85	0.94	57,57,57,57	0
56	MG	1a	1662	1/1	0.85	0.20	62,62,62,62	0
56	MG	2A	3568	1/1	0.85	0.18	57,57,57,57	0
56	MG	2A	3792	1/1	0.85	0.13	90,90,90,90	0
56	MG	1A	3186	1/1	0.85	0.12	58,58,58,58	0
56	MG	2A	3412	1/1	0.85	0.14	57,57,57,57	0
56	MG	2a	1613	1/1	0.85	0.26	52,52,52,52	0
56	MG	2A	3801	1/1	0.85	0.27	86,86,86,86	0
56	MG	2A	3577	1/1	0.85	0.15	31,31,31,31	0
56	MG	2A	3144	1/1	0.85	0.36	62,62,62,62	0
56	MG	2A	3311	1/1	0.85	0.13	61,61,61,61	0
56	MG	1a	1708	1/1	0.85	0.16	64,64,64,64	0
56	MG	2A	3587	1/1	0.85	0.16	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	3427	1/1	0.85	0.18	52,52,52,52	0
56	MG	1A	3428	1/1	0.85	0.38	41,41,41,41	0
56	MG	2q	203	1/1	0.85	0.14	75,75,75,75	0
56	MG	1A	4106	1/1	0.85	0.08	52,52,52,52	0
56	MG	1A	4115	1/1	0.85	0.92	72,72,72,72	0
56	MG	1A	3375	1/1	0.85	0.97	37,37,37,37	0
56	MG	1A	3450	1/1	0.85	0.12	56,56,56,56	0
56	MG	1A	3539	1/1	0.85	0.28	61,61,61,61	0
56	MG	2A	3191	1/1	0.85	0.37	72,72,72,72	0
56	MG	2A	3625	1/1	0.85	0.17	72,72,72,72	0
56	MG	2A	3545	1/1	0.86	0.11	47,47,47,47	0
56	MG	1A	3622	1/1	0.86	0.13	68,68,68,68	0
56	MG	2A	3555	1/1	0.86	0.09	55,55,55,55	0
56	MG	2A	3558	1/1	0.86	0.15	51,51,51,51	0
56	MG	1A	4068	1/1	0.86	0.06	54,54,54,54	0
56	MG	1a	1692	1/1	0.86	0.21	52,52,52,52	0
56	MG	2A	3565	1/1	0.86	0.15	56,56,56,56	0
56	MG	1A	3873	1/1	0.86	0.17	22,22,22,22	0
56	MG	2A	3800	1/1	0.86	0.30	63,63,63,63	0
56	MG	2A	3293	1/1	0.86	0.71	64,64,64,64	0
56	MG	1a	1719	1/1	0.86	0.19	85,85,85,85	0
56	MG	1A	3751	1/1	0.86	0.14	21,21,21,21	0
56	MG	2A	3803	1/1	0.86	0.17	71,71,71,71	0
56	MG	2A	3141	1/1	0.86	0.17	50,50,50,50	0
56	MG	1A	3755	1/1	0.86	0.12	31,31,31,31	0
56	MG	1A	3976	1/1	0.86	0.07	66,66,66,66	0
56	MG	1A	4112	1/1	0.86	0.74	36,36,36,36	0
56	MG	2A	3593	1/1	0.86	0.14	35,35,35,35	0
56	MG	2A	3154	1/1	0.86	0.13	63,63,63,63	0
56	MG	2A	3163	1/1	0.86	0.21	76,76,76,76	0
56	MG	1A	3433	1/1	0.86	0.47	62,62,62,62	0
56	MG	2A	3423	1/1	0.86	0.13	70,70,70,70	0
56	MG	2A	3832	1/1	0.86	0.06	53,53,53,53	0
56	MG	1A	4125	1/1	0.86	0.40	35,35,35,35	0
56	MG	2A	3313	1/1	0.86	0.08	62,62,62,62	0
56	MG	1A	3630	1/1	0.86	0.17	33,33,33,33	0
56	MG	2A	3176	1/1	0.86	0.10	61,61,61,61	0
56	MG	2a	1695	1/1	0.86	0.19	65,65,65,65	0
56	MG	1A	4141	1/1	0.86	0.12	44,44,44,44	0
56	MG	2A	3626	1/1	0.86	0.13	31,31,31,31	0
56	MG	2a	1702	1/1	0.86	0.14	69,69,69,69	0
56	MG	2A	3856	1/1	0.86	0.49	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3894	1/1	0.86	0.15	53,53,53,53	0
56	MG	2A	3189	1/1	0.86	0.16	69,69,69,69	0
56	MG	1B	209	1/1	0.86	0.14	57,57,57,57	0
56	MG	1A	3514	1/1	0.86	0.09	56,56,56,56	0
56	MG	1A	3788	1/1	0.86	0.09	38,38,38,38	0
56	MG	2A	3448	1/1	0.86	1.03	64,64,64,64	0
56	MG	1A	3306	1/1	0.86	0.18	54,54,54,54	0
56	MG	1A	3996	1/1	0.86	0.10	20,20,20,20	0
56	MG	1A	3415	1/1	0.86	0.20	59,59,59,59	0
56	MG	2A	3659	1/1	0.86	0.10	31,31,31,31	0
56	MG	1A	3486	1/1	0.86	0.38	47,47,47,47	0
56	MG	2A	3220	1/1	0.86	0.14	48,48,48,48	0
56	MG	1D	311	1/1	0.86	0.63	41,41,41,41	0
56	MG	2A	3346	1/1	0.86	0.16	60,60,60,60	0
56	MG	1A	3917	1/1	0.86	0.14	31,31,31,31	0
56	MG	2A	3685	1/1	0.86	0.11	63,63,63,63	0
56	MG	1G	201	1/1	0.86	0.16	37,37,37,37	0
56	MG	1A	3390	1/1	0.86	0.71	38,38,38,38	0
56	MG	2a	1754	1/1	0.86	0.08	57,57,57,57	0
56	MG	1A	3663	1/1	0.86	0.35	61,61,61,61	0
56	MG	1A	3202	1/1	0.86	0.09	25,25,25,25	0
56	MG	2A	3236	1/1	0.86	0.19	59,59,59,59	0
56	MG	1A	3584	1/1	0.86	0.17	50,50,50,50	0
56	MG	1l	202	1/1	0.86	0.21	83,83,83,83	0
56	MG	1A	3936	1/1	0.86	0.09	62,62,62,62	0
56	MG	2A	3484	1/1	0.86	0.33	54,54,54,54	0
56	MG	1T	202	1/1	0.86	0.14	45,45,45,45	0
56	MG	1x	102	1/1	0.86	0.20	57,57,57,57	0
56	MG	1A	3817	1/1	0.86	0.12	56,56,56,56	0
56	MG	1U	206	1/1	0.86	1.53	70,70,70,70	0
56	MG	2a	1782	1/1	0.86	0.26	72,72,72,72	0
56	MG	1X	103	1/1	0.86	0.34	40,40,40,40	0
56	MG	2A	3714	1/1	0.86	0.13	71,71,71,71	0
56	MG	2A	3718	1/1	0.86	0.24	70,70,70,70	0
56	MG	2A	3359	1/1	0.86	0.15	58,58,58,58	0
56	MG	1A	3019	1/1	0.86	0.13	48,48,48,48	0
56	MG	2A	3365	1/1	0.86	0.61	45,45,45,45	0
56	MG	1A	4018	1/1	0.86	0.10	47,47,47,47	0
56	MG	2A	3257	1/1	0.86	0.13	55,55,55,55	0
56	MG	1A	3676	1/1	0.86	0.15	50,50,50,50	0
56	MG	13	103	1/1	0.86	0.13	59,59,59,59	0
56	MG	2A	3069	1/1	0.86	0.23	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	3741	1/1	0.86	0.08	49,49,49,49	0
56	MG	2A	3501	1/1	0.86	0.16	48,48,48,48	0
56	MG	2E	306	1/1	0.86	0.10	47,47,47,47	0
56	MG	2A	3262	1/1	0.86	0.49	54,54,54,54	0
56	MG	1A	3823	1/1	0.86	0.29	40,40,40,40	0
56	MG	2F	304	1/1	0.86	0.10	58,58,58,58	0
56	MG	1A	3465	1/1	0.86	0.22	64,64,64,64	0
56	MG	1a	1625	1/1	0.86	0.24	57,57,57,57	0
56	MG	2A	3752	1/1	0.86	0.10	46,46,46,46	0
56	MG	1A	3535	1/1	0.86	0.21	56,56,56,56	0
56	MG	1a	1632	1/1	0.86	0.26	62,62,62,62	0
56	MG	2a	1831	1/1	0.86	0.20	80,80,80,80	0
56	MG	1A	3403	1/1	0.86	0.20	46,46,46,46	0
56	MG	2W	201	1/1	0.86	0.26	60,60,60,60	0
56	MG	1A	3355	1/1	0.86	0.55	61,61,61,61	0
56	MG	2A	3516	1/1	0.86	0.48	49,49,49,49	0
56	MG	1A	3193	1/1	0.86	0.90	41,41,41,41	0
56	MG	1A	3711	1/1	0.86	0.15	39,39,39,39	0
56	MG	1A	3504	1/1	0.86	0.50	57,57,57,57	0
56	MG	2A	3775	1/1	0.86	0.15	59,59,59,59	0
56	MG	1A	3868	1/1	0.86	0.72	38,38,38,38	0
56	MG	1A	3088	1/1	0.86	0.30	38,38,38,38	0
56	MG	2a	1617	1/1	0.86	0.80	73,73,73,73	0
56	MG	2A	3284	1/1	0.86	1.43	48,48,48,48	0
56	MG	2a	1623	1/1	0.86	0.17	56,56,56,56	0
56	MG	2A	3785	1/1	0.86	0.27	65,65,65,65	0
56	MG	1A	3291	1/1	0.87	0.17	66,66,66,66	0
56	MG	2A	3160	1/1	0.87	0.13	49,49,49,49	0
56	MG	1A	3092	1/1	0.87	0.16	43,43,43,43	0
56	MG	2a	1674	1/1	0.87	0.07	59,59,59,59	0
56	MG	2A	3621	1/1	0.87	0.59	55,55,55,55	0
56	MG	2A	3005	1/1	0.87	0.25	49,49,49,49	0
56	MG	1A	3244	1/1	0.87	0.30	60,60,60,60	0
56	MG	1A	3793	1/1	0.87	0.17	24,24,24,24	0
56	MG	2A	3627	1/1	0.87	0.21	52,52,52,52	0
56	MG	2A	3380	1/1	0.87	0.30	57,57,57,57	0
56	MG	2A	3026	1/1	0.87	0.39	53,53,53,53	0
56	MG	2A	3482	1/1	0.87	0.23	60,60,60,60	0
56	MG	2A	3384	1/1	0.87	0.42	41,41,41,41	0
56	MG	2A	3385	1/1	0.87	0.41	70,70,70,70	0
56	MG	1A	3247	1/1	0.87	0.11	67,67,67,67	0
56	MG	2A	3807	1/1	0.87	0.11	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	1t	201	1/1	0.87	0.13	56,56,56,56	0
56	MG	1A	3462	1/1	0.87	0.55	54,54,54,54	0
56	MG	1A	3968	1/1	0.87	0.15	52,52,52,52	0
56	MG	1a	1628	1/1	0.87	0.22	55,55,55,55	0
56	MG	1A	3356	1/1	0.87	0.32	46,46,46,46	0
56	MG	1A	4040	1/1	0.87	0.20	54,54,54,54	0
56	MG	2A	3671	1/1	0.87	0.48	63,63,63,63	0
56	MG	2A	3819	1/1	0.87	0.14	31,31,31,31	0
56	MG	2A	3194	1/1	0.87	0.36	61,61,61,61	0
56	MG	2a	1734	1/1	0.87	0.14	57,57,57,57	0
56	MG	2A	3041	1/1	0.87	0.11	68,68,68,68	0
56	MG	1A	3677	1/1	0.87	0.13	22,22,22,22	0
56	MG	1a	1646	1/1	0.87	0.23	50,50,50,50	0
56	MG	1A	3285	1/1	0.87	0.21	41,41,41,41	0
56	MG	1A	3599	1/1	0.87	0.20	23,23,23,23	0
56	MG	1A	3378	1/1	0.87	0.62	40,40,40,40	0
56	MG	2A	3837	1/1	0.87	0.14	61,61,61,61	0
56	MG	1A	3333	1/1	0.87	0.12	53,53,53,53	0
56	MG	2A	3062	1/1	0.87	0.13	63,63,63,63	0
56	MG	2A	3513	1/1	0.87	0.20	61,61,61,61	0
56	MG	1a	1671	1/1	0.87	0.15	53,53,53,53	0
56	MG	2B	219	1/1	0.87	0.26	77,77,77,77	0
56	MG	2A	3841	1/1	0.87	0.16	39,39,39,39	0
56	MG	1A	3605	1/1	0.87	0.12	47,47,47,47	0
56	MG	2A	3230	1/1	0.87	0.13	55,55,55,55	0
56	MG	2A	3858	1/1	0.87	0.11	66,66,66,66	0
56	MG	2A	3702	1/1	0.87	0.20	73,73,73,73	0
56	MG	2a	1766	1/1	0.87	0.20	60,60,60,60	0
56	MG	2A	3410	1/1	0.87	0.33	70,70,70,70	0
56	MG	1A	3339	1/1	0.87	0.13	57,57,57,57	0
56	MG	2a	1773	1/1	0.87	0.22	73,73,73,73	0
56	MG	1A	4065	1/1	0.87	0.20	52,52,52,52	0
56	MG	2R	201	1/1	0.87	0.63	78,78,78,78	0
56	MG	1a	1714	1/1	0.87	0.14	71,71,71,71	0
56	MG	1A	3829	1/1	0.87	0.09	39,39,39,39	0
56	MG	1B	217	1/1	0.87	0.11	50,50,50,50	0
56	MG	2A	3728	1/1	0.87	0.21	52,52,52,52	0
56	MG	2A	3417	1/1	0.87	0.28	57,57,57,57	0
56	MG	1A	3612	1/1	0.87	0.14	35,35,35,35	0
56	MG	2a	1604	1/1	0.87	0.15	50,50,50,50	0
56	MG	2A	3539	1/1	0.87	0.14	50,50,50,50	0
56	MG	1A	4084	1/1	0.87	0.24	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	1B	231	1/1	0.87	0.11	64,64,64,64	0
56	MG	2A	3339	1/1	0.87	0.11	58,58,58,58	0
56	MG	1A	3265	1/1	0.87	0.24	48,48,48,48	0
56	MG	1D	307	1/1	0.87	0.23	37,37,37,37	0
56	MG	2A	3254	1/1	0.87	0.16	59,59,59,59	0
56	MG	1A	4092	1/1	0.87	0.17	60,60,60,60	0
56	MG	1a	1760	1/1	0.87	0.19	58,58,58,58	0
56	MG	1A	3342	1/1	0.87	0.74	37,37,37,37	0
56	MG	1A	4099	1/1	0.87	0.13	63,63,63,63	0
56	MG	1A	3266	1/1	0.87	0.12	59,59,59,59	0
56	MG	1a	1772	1/1	0.87	0.17	53,53,53,53	0
56	MG	1A	4004	1/1	0.87	0.11	38,38,38,38	0
56	MG	1G	204	1/1	0.87	0.13	42,42,42,42	0
56	MG	1A	3561	1/1	0.87	0.14	34,34,34,34	0
56	MG	2e	201	1/1	0.87	0.10	79,79,79,79	0
56	MG	2a	1645	1/1	0.87	0.15	57,57,57,57	0
56	MG	1A	4006	1/1	0.87	0.08	74,74,74,74	0
56	MG	2a	1648	1/1	0.87	1.06	81,81,81,81	0
56	MG	1a	1780	1/1	0.87	0.10	64,64,64,64	0
56	MG	1A	3860	1/1	0.87	0.10	29,29,29,29	0
56	MG	1A	3562	1/1	0.87	0.73	48,48,48,48	0
56	MG	2A	3590	1/1	0.87	0.11	54,54,54,54	0
56	MG	1A	3090	1/1	0.87	0.22	46,46,46,46	0
56	MG	2a	1658	1/1	0.87	0.17	73,73,73,73	0
56	MG	2x	102	1/1	0.87	0.08	75,75,75,75	0
56	MG	2A	3273	1/1	0.87	0.72	47,47,47,47	0
56	MG	1A	3766	1/1	0.87	0.13	38,38,38,38	0
56	MG	1U	205	1/1	0.87	0.28	49,49,49,49	0
56	MG	2y	106	1/1	0.87	0.17	84,84,84,84	0
56	MG	2A	3363	1/1	0.87	0.17	55,55,55,55	0
56	MG	1A	3434	1/1	0.87	0.15	63,63,63,63	0
56	MG	1A	3830	1/1	0.88	0.21	53,53,53,53	0
56	MG	1a	1738	1/1	0.88	0.11	59,59,59,59	0
56	MG	2a	1644	1/1	0.88	0.16	55,55,55,55	0
56	MG	1A	3833	1/1	0.88	0.05	46,46,46,46	0
56	MG	1A	4021	1/1	0.88	0.25	69,69,69,69	0
56	MG	2A	3662	1/1	0.88	0.07	40,40,40,40	0
56	MG	1A	4026	1/1	0.88	0.13	56,56,56,56	0
56	MG	1A	3944	1/1	0.88	0.28	82,82,82,82	0
56	MG	1A	4029	1/1	0.88	0.12	38,38,38,38	0
56	MG	2A	3478	1/1	0.88	0.23	62,62,62,62	0
56	MG	1A	3710	1/1	0.88	0.07	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	2A	3237	1/1	0.88	0.80	68,68,68,68	0
56	MG	1A	3837	1/1	0.88	0.10	54,54,54,54	0
56	MG	1B	212	1/1	0.88	0.14	51,51,51,51	0
56	MG	1A	3074	1/1	0.88	0.25	58,58,58,58	0
56	MG	2A	3250	1/1	0.88	0.13	67,67,67,67	0
56	MG	2A	3251	1/1	0.88	0.17	64,64,64,64	0
56	MG	2A	3490	1/1	0.88	0.32	40,40,40,40	0
56	MG	1A	3041	1/1	0.88	0.10	31,31,31,31	0
56	MG	1B	227	1/1	0.88	0.15	45,45,45,45	0
56	MG	1A	3847	1/1	0.88	0.11	46,46,46,46	0
56	MG	1a	1779	1/1	0.88	0.23	72,72,72,72	0
56	MG	1A	3731	1/1	0.88	0.09	33,33,33,33	0
56	MG	2A	3706	1/1	0.88	0.16	66,66,66,66	0
56	MG	1A	4047	1/1	0.88	0.10	41,41,41,41	0
56	MG	1B	237	1/1	0.88	0.13	37,37,37,37	0
56	MG	1A	3608	1/1	0.88	0.23	36,36,36,36	0
56	MG	1A	3466	1/1	0.88	0.10	66,66,66,66	0
56	MG	2A	3719	1/1	0.88	0.14	90,90,90,90	0
56	MG	2A	3723	1/1	0.88	0.12	26,26,26,26	0
56	MG	2A	3724	1/1	0.88	0.19	86,86,86,86	0
56	MG	1A	3391	1/1	0.88	0.27	56,56,56,56	0
56	MG	2A	3102	1/1	0.88	0.18	43,43,43,43	0
56	MG	1a	1804	1/1	0.88	0.14	66,66,66,66	0
56	MG	1a	1805	1/1	0.88	0.10	60,60,60,60	0
56	MG	2a	1713	1/1	0.88	0.12	86,86,86,86	0
56	MG	1A	3105	1/1	0.88	1.05	37,37,37,37	0
56	MG	1A	3756	1/1	0.88	0.22	26,26,26,26	0
56	MG	2A	3111	1/1	0.88	0.10	55,55,55,55	0
56	MG	2a	1720	1/1	0.88	0.16	55,55,55,55	0
56	MG	1A	3558	1/1	0.88	0.13	53,53,53,53	0
56	MG	2A	3738	1/1	0.88	0.10	55,55,55,55	0
56	MG	1A	3369	1/1	0.88	0.28	44,44,44,44	0
56	MG	2a	1731	1/1	0.88	0.14	72,72,72,72	0
56	MG	2a	1732	1/1	0.88	0.19	62,62,62,62	0
56	MG	1A	3472	1/1	0.88	0.30	44,44,44,44	0
56	MG	1a	1826	1/1	0.88	0.15	62,62,62,62	0
56	MG	1A	3183	1/1	0.88	0.09	39,39,39,39	0
56	MG	1a	1831	1/1	0.88	0.08	69,69,69,69	0
56	MG	1A	3884	1/1	0.88	0.12	22,22,22,22	0
56	MG	2A	3127	1/1	0.88	0.26	53,53,53,53	0
56	MG	1A	4088	1/1	0.88	0.09	50,50,50,50	0
56	MG	2A	3281	1/1	0.88	0.12	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	2a	1744	1/1	0.88	0.14	65,65,65,65	0
56	MG	2A	3751	1/1	0.88	0.10	66,66,66,66	0
56	MG	2a	1748	1/1	0.88	0.10	56,56,56,56	0
56	MG	1Y	201	1/1	0.88	0.14	44,44,44,44	0
56	MG	1A	4091	1/1	0.88	0.16	61,61,61,61	0
56	MG	2A	3283	1/1	0.88	0.16	75,75,75,75	0
56	MG	2A	3754	1/1	0.88	0.16	67,67,67,67	0
56	MG	1A	3648	1/1	0.88	0.12	62,62,62,62	0
56	MG	2A	3547	1/1	0.88	0.17	73,73,73,73	0
56	MG	1A	3316	1/1	0.88	1.56	44,44,44,44	0
56	MG	1A	3889	1/1	0.88	0.16	58,58,58,58	0
56	MG	1A	4100	1/1	0.88	0.13	29,29,29,29	0
56	MG	2A	3769	1/1	0.88	0.26	60,60,60,60	0
56	MG	2A	3771	1/1	0.88	0.12	55,55,55,55	0
56	MG	2A	3407	1/1	0.88	0.41	51,51,51,51	0
56	MG	15	105	1/1	0.88	0.29	36,36,36,36	0
56	MG	1A	3567	1/1	0.88	0.58	35,35,35,35	0
56	MG	2a	1775	1/1	0.88	0.10	49,49,49,49	0
56	MG	2a	1777	1/1	0.88	0.14	68,68,68,68	0
56	MG	18	102	1/1	0.88	0.16	38,38,38,38	0
56	MG	1A	4110	1/1	0.88	0.71	36,36,36,36	0
56	MG	1A	3896	1/1	0.88	0.21	52,52,52,52	0
56	MG	1A	3332	1/1	0.88	0.18	43,43,43,43	0
56	MG	2B	213	1/1	0.88	0.31	69,69,69,69	0
56	MG	2A	3576	1/1	0.88	0.13	49,49,49,49	0
56	MG	2B	215	1/1	0.88	0.21	75,75,75,75	0
56	MG	1A	3580	1/1	0.88	0.22	41,41,41,41	0
56	MG	1A	3481	1/1	0.88	0.27	51,51,51,51	0
56	MG	1A	3407	1/1	0.88	0.18	45,45,45,45	0
56	MG	1a	1631	1/1	0.88	0.29	71,71,71,71	0
56	MG	1A	3483	1/1	0.88	0.11	61,61,61,61	0
56	MG	2A	3174	1/1	0.88	0.17	63,63,63,63	0
56	MG	1A	3805	1/1	0.88	0.11	55,55,55,55	0
56	MG	2A	3796	1/1	0.88	0.10	69,69,69,69	0
56	MG	1A	3139	1/1	0.88	0.29	43,43,43,43	0
56	MG	1A	3487	1/1	0.88	0.49	45,45,45,45	0
56	MG	1A	4149	1/1	0.88	0.37	32,32,32,32	0
56	MG	1A	3454	1/1	0.88	0.82	37,37,37,37	0
56	MG	1A	3146	1/1	0.88	0.28	39,39,39,39	0
56	MG	1a	1659	1/1	0.88	0.18	62,62,62,62	0
56	MG	2A	3612	1/1	0.88	0.19	68,68,68,68	0
56	MG	1A	3382	1/1	0.88	0.22	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	3324	1/1	0.88	0.22	73,73,73,73	0
56	MG	2A	3195	1/1	0.88	0.28	71,71,71,71	0
56	MG	28	101	1/1	0.88	0.12	49,49,49,49	0
56	MG	2A	3015	1/1	0.88	0.21	52,52,52,52	0
56	MG	2a	1605	1/1	0.88	0.13	72,72,72,72	0
56	MG	1a	1670	1/1	0.88	0.14	49,49,49,49	0
56	MG	2A	3446	1/1	0.88	0.40	72,72,72,72	0
56	MG	2A	3202	1/1	0.88	0.12	63,63,63,63	0
56	MG	2A	3818	1/1	0.88	0.14	42,42,42,42	0
56	MG	2A	3449	1/1	0.88	0.28	57,57,57,57	0
56	MG	2A	3330	1/1	0.88	0.28	60,60,60,60	0
56	MG	2A	3207	1/1	0.88	0.18	34,34,34,34	0
56	MG	2A	3824	1/1	0.88	0.13	34,34,34,34	0
56	MG	2x	103	1/1	0.88	0.09	78,78,78,78	0
56	MG	2A	3828	1/1	0.88	0.13	43,43,43,43	0
56	MG	2A	3213	1/1	0.88	0.16	60,60,60,60	0
56	MG	2A	3638	1/1	0.88	0.14	25,25,25,25	0
56	MG	1A	3692	1/1	0.88	0.13	53,53,53,53	0
56	MG	2A	3023	1/1	0.88	0.13	42,42,42,42	0
56	MG	1A	3386	1/1	0.88	0.48	29,29,29,29	0
56	MG	2A	3400	1/1	0.89	0.18	44,44,44,44	0
56	MG	1A	3973	1/1	0.89	0.17	20,20,20,20	0
56	MG	2A	3531	1/1	0.89	0.10	40,40,40,40	0
56	MG	1D	312	1/1	0.89	0.38	23,23,23,23	0
56	MG	1A	3899	1/1	0.89	0.56	37,37,37,37	0
56	MG	1a	1776	1/1	0.89	0.23	80,80,80,80	0
56	MG	2A	3299	1/1	0.89	0.32	69,69,69,69	0
56	MG	2A	3543	1/1	0.89	0.16	35,35,35,35	0
56	MG	2A	3188	1/1	0.89	0.08	72,72,72,72	0
56	MG	2A	3038	1/1	0.89	0.22	41,41,41,41	0
56	MG	1A	3904	1/1	0.89	0.15	43,43,43,43	0
56	MG	2A	3192	1/1	0.89	0.28	59,59,59,59	0
56	MG	1A	3700	1/1	0.89	0.16	34,34,34,34	0
56	MG	1A	3408	1/1	0.89	0.21	53,53,53,53	0
56	MG	1A	3910	1/1	0.89	0.25	72,72,72,72	0
56	MG	1A	4064	1/1	0.89	0.06	48,48,48,48	0
56	MG	2A	3418	1/1	0.89	0.47	66,66,66,66	0
56	MG	1A	3453	1/1	0.89	0.22	49,49,49,49	0
56	MG	1A	3983	1/1	0.89	0.11	37,37,37,37	0
56	MG	1U	203	1/1	0.89	0.74	42,42,42,42	0
56	MG	1A	4070	1/1	0.89	0.12	51,51,51,51	0
56	MG	2a	1688	1/1	0.89	0.13	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	3767	1/1	0.89	0.14	34,34,34,34	0
56	MG	2A	3768	1/1	0.89	1.02	46,46,46,46	0
56	MG	2a	1693	1/1	0.89	0.16	46,46,46,46	0
56	MG	1a	1810	1/1	0.89	0.09	59,59,59,59	0
56	MG	1A	3826	1/1	0.89	0.10	57,57,57,57	0
56	MG	2A	3583	1/1	0.89	0.09	37,37,37,37	0
56	MG	2a	1701	1/1	0.89	0.13	56,56,56,56	0
56	MG	2A	3064	1/1	0.89	0.22	66,66,66,66	0
56	MG	1A	3409	1/1	0.89	0.15	63,63,63,63	0
56	MG	1a	1822	1/1	0.89	0.08	69,69,69,69	0
56	MG	2A	3326	1/1	0.89	0.35	56,56,56,56	0
56	MG	2A	3433	1/1	0.89	0.30	62,62,62,62	0
56	MG	2A	3070	1/1	0.89	0.11	58,58,58,58	0
56	MG	1A	3916	1/1	0.89	0.18	22,22,22,22	0
56	MG	2A	3601	1/1	0.89	0.18	45,45,45,45	0
56	MG	1A	3572	1/1	0.89	0.56	37,37,37,37	0
56	MG	1A	4000	1/1	0.89	0.11	36,36,36,36	0
56	MG	1A	3636	1/1	0.89	0.15	21,21,21,21	0
56	MG	2A	3233	1/1	0.89	0.12	78,78,78,78	0
56	MG	1h	201	1/1	0.89	0.24	64,64,64,64	0
56	MG	2a	1730	1/1	0.89	0.10	66,66,66,66	0
56	MG	1l	201	1/1	0.89	0.20	42,42,42,42	0
56	MG	1A	3025	1/1	0.89	0.15	42,42,42,42	0
56	MG	1m	202	1/1	0.89	0.11	56,56,56,56	0
56	MG	1r	101	1/1	0.89	0.11	70,70,70,70	0
56	MG	2A	3342	1/1	0.89	0.15	41,41,41,41	0
56	MG	1a	1603	1/1	0.89	0.12	50,50,50,50	0
56	MG	2A	3343	1/1	0.89	0.14	66,66,66,66	0
56	MG	1a	1606	1/1	0.89	0.12	50,50,50,50	0
56	MG	2A	3107	1/1	0.89	0.14	62,62,62,62	0
56	MG	2a	1742	1/1	0.89	0.17	77,77,77,77	0
56	MG	1A	3360	1/1	0.89	0.40	38,38,38,38	0
56	MG	1a	1619	1/1	0.89	0.19	48,48,48,48	0
56	MG	1x	112	1/1	0.89	0.29	65,65,65,65	0
56	MG	1a	1624	1/1	0.89	0.22	47,47,47,47	0
56	MG	1A	3643	1/1	0.89	0.10	37,37,37,37	0
56	MG	2A	3114	1/1	0.89	0.14	41,41,41,41	0
56	MG	1A	3583	1/1	0.89	0.15	65,65,65,65	0
56	MG	1A	3020	1/1	0.89	0.16	38,38,38,38	0
56	MG	1A	3490	1/1	0.89	0.52	45,45,45,45	0
56	MG	1A	3660	1/1	0.89	0.13	21,21,21,21	0
56	MG	1A	4124	1/1	0.89	0.22	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	4014	1/1	0.89	0.24	60,60,60,60	0
56	MG	2A	3128	1/1	0.89	0.08	70,70,70,70	0
56	MG	1A	3166	1/1	0.89	0.18	51,51,51,51	0
56	MG	2a	1765	1/1	0.89	0.10	69,69,69,69	0
56	MG	1A	3295	1/1	0.89	0.36	64,64,64,64	0
56	MG	2A	3479	1/1	0.89	0.21	54,54,54,54	0
56	MG	1a	1654	1/1	0.89	0.29	68,68,68,68	0
56	MG	1A	3771	1/1	0.89	0.12	41,41,41,41	0
56	MG	2A	3364	1/1	0.89	0.12	51,51,51,51	0
56	MG	2D	301	1/1	0.89	0.11	34,34,34,34	0
56	MG	2A	3265	1/1	0.89	0.28	53,53,53,53	0
56	MG	2A	3674	1/1	0.89	0.66	49,49,49,49	0
56	MG	1A	4143	1/1	0.89	0.11	51,51,51,51	0
56	MG	2A	3139	1/1	0.89	0.70	51,51,51,51	0
56	MG	2A	3679	1/1	0.89	0.44	55,55,55,55	0
56	MG	1A	3298	1/1	0.89	0.28	51,51,51,51	0
56	MG	2a	1797	1/1	0.89	0.09	62,62,62,62	0
56	MG	2A	3372	1/1	0.89	0.22	50,50,50,50	0
56	MG	2A	3493	1/1	0.89	0.17	49,49,49,49	0
56	MG	1A	3271	1/1	0.89	0.80	49,49,49,49	0
56	MG	2a	1803	1/1	0.89	0.13	66,66,66,66	0
56	MG	2A	3145	1/1	0.89	0.64	57,57,57,57	0
56	MG	2T	202	1/1	0.89	0.14	51,51,51,51	0
56	MG	2U	201	1/1	0.89	0.15	44,44,44,44	0
56	MG	1A	3064	1/1	0.89	0.23	57,57,57,57	0
56	MG	2A	3850	1/1	0.89	0.46	51,51,51,51	0
56	MG	1A	3307	1/1	0.89	0.38	42,42,42,42	0
56	MG	2X	101	1/1	0.89	0.17	47,47,47,47	0
56	MG	2A	3276	1/1	0.89	0.19	64,64,64,64	0
56	MG	2A	3860	1/1	0.89	0.19	36,36,36,36	0
56	MG	1A	3115	1/1	0.89	0.09	41,41,41,41	0
56	MG	2A	3158	1/1	0.89	0.13	60,60,60,60	0
56	MG	1A	3206	1/1	0.89	0.48	54,54,54,54	0
56	MG	2A	3162	1/1	0.89	0.17	70,70,70,70	0
56	MG	2A	3712	1/1	0.89	0.15	79,79,79,79	0
56	MG	2a	1826	1/1	0.89	0.37	75,75,75,75	0
56	MG	1A	3680	1/1	0.89	0.14	21,21,21,21	0
56	MG	1A	3142	1/1	0.89	0.45	43,43,43,43	0
56	MG	1A	3212	1/1	0.89	0.17	54,54,54,54	0
56	MG	1B	221	1/1	0.89	0.11	50,50,50,50	0
56	MG	1A	3691	1/1	0.89	0.21	24,24,24,24	0
56	MG	2A	3289	1/1	0.89	0.17	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1a	1746	1/1	0.89	0.22	62,62,62,62	0
56	MG	1a	1747	1/1	0.89	0.17	49,49,49,49	0
56	MG	1A	3442	1/1	0.89	0.44	40,40,40,40	0
56	MG	2a	1629	1/1	0.89	0.69	62,62,62,62	0
56	MG	2A	3520	1/1	0.89	0.15	40,40,40,40	0
56	MG	1A	3820	1/1	0.89	0.16	59,59,59,59	0
56	MG	2a	1636	1/1	0.89	0.28	49,49,49,49	0
56	MG	2A	3177	1/1	0.89	0.25	59,59,59,59	0
56	MG	2a	1640	1/1	0.89	0.20	62,62,62,62	0
56	MG	1B	233	1/1	0.89	0.13	57,57,57,57	0
56	MG	1B	234	1/1	0.89	0.40	67,67,67,67	0
56	MG	2a	1643	1/1	0.89	0.14	75,75,75,75	0
56	MG	2A	3732	1/1	0.89	0.24	62,62,62,62	0
58	K	2A	3515	1/1	0.89	0.08	66,66,66,66	0
56	MG	2A	3525	1/1	0.89	0.31	62,62,62,62	0
56	MG	1A	3947	1/1	0.90	0.09	53,53,53,53	0
56	MG	1A	3670	1/1	0.90	0.10	18,18,18,18	0
56	MG	2A	3503	1/1	0.90	0.13	60,60,60,60	0
56	MG	2A	3263	1/1	0.90	0.31	60,60,60,60	0
56	MG	1A	3441	1/1	0.90	0.51	40,40,40,40	0
56	MG	1A	3392	1/1	0.90	0.35	51,51,51,51	0
56	MG	1A	3445	1/1	0.90	0.27	51,51,51,51	0
56	MG	2A	3510	1/1	0.90	0.41	65,65,65,65	0
56	MG	2A	3512	1/1	0.90	0.15	56,56,56,56	0
56	MG	2A	3268	1/1	0.90	0.68	53,53,53,53	0
56	MG	1A	3573	1/1	0.90	0.29	49,49,49,49	0
56	MG	2a	1655	1/1	0.90	0.68	63,63,63,63	0
56	MG	1A	4083	1/1	0.90	0.31	55,55,55,55	0
56	MG	1A	3448	1/1	0.90	0.25	65,65,65,65	0
56	MG	1E	303	1/1	0.90	0.47	36,36,36,36	0
56	MG	2A	3733	1/1	0.90	0.33	66,66,66,66	0
56	MG	1F	302	1/1	0.90	0.14	53,53,53,53	0
56	MG	1A	3286	1/1	0.90	0.16	59,59,59,59	0
56	MG	2A	3388	1/1	0.90	0.15	50,50,50,50	0
56	MG	2A	3523	1/1	0.90	0.64	36,36,36,36	0
56	MG	1G	202	1/1	0.90	0.27	61,61,61,61	0
56	MG	1A	3322	1/1	0.90	0.13	41,41,41,41	0
56	MG	2A	3133	1/1	0.90	0.60	57,57,57,57	0
56	MG	1G	205	1/1	0.90	0.13	54,54,54,54	0
56	MG	1A	3963	1/1	0.90	0.10	59,59,59,59	0
56	MG	2a	1683	1/1	0.90	0.15	72,72,72,72	0
56	MG	2A	3137	1/1	0.90	0.17	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	3964	1/1	0.90	0.40	77,77,77,77	0
56	MG	1a	1802	1/1	0.90	0.12	83,83,83,83	0
56	MG	1A	3683	1/1	0.90	0.14	13,13,13,13	0
56	MG	2A	3748	1/1	0.90	0.09	68,68,68,68	0
56	MG	2A	3535	1/1	0.90	0.20	35,35,35,35	0
56	MG	1R	202	1/1	0.90	0.14	35,35,35,35	0
56	MG	1A	3400	1/1	0.90	0.38	53,53,53,53	0
56	MG	1A	3510	1/1	0.90	0.26	54,54,54,54	0
56	MG	1A	3844	1/1	0.90	0.15	16,16,16,16	0
56	MG	1A	3323	1/1	0.90	0.22	42,42,42,42	0
56	MG	2A	3550	1/1	0.90	0.19	52,52,52,52	0
56	MG	1X	101	1/1	0.90	0.21	34,34,34,34	0
56	MG	1A	3693	1/1	0.90	0.17	24,24,24,24	0
56	MG	2A	3757	1/1	0.90	0.13	39,39,39,39	0
56	MG	1A	3328	1/1	0.90	0.10	56,56,56,56	0
56	MG	2a	1717	1/1	0.90	0.08	52,52,52,52	0
56	MG	1a	1829	1/1	0.90	0.10	62,62,62,62	0
56	MG	2A	3763	1/1	0.90	0.10	59,59,59,59	0
56	MG	1A	3977	1/1	0.90	0.20	38,38,38,38	0
56	MG	1A	3516	1/1	0.90	0.36	45,45,45,45	0
56	MG	2a	1722	1/1	0.90	0.11	49,49,49,49	0
56	MG	1A	3709	1/1	0.90	0.19	46,46,46,46	0
56	MG	1a	1838	1/1	0.90	0.14	58,58,58,58	0
56	MG	2a	1728	1/1	0.90	0.23	74,74,74,74	0
56	MG	1a	1839	1/1	0.90	0.07	76,76,76,76	0
56	MG	1A	3865	1/1	0.90	0.63	54,54,54,54	0
56	MG	1A	3329	1/1	0.90	0.14	50,50,50,50	0
56	MG	1A	3521	1/1	0.90	0.75	44,44,44,44	0
56	MG	13	101	1/1	0.90	0.27	56,56,56,56	0
56	MG	2A	3772	1/1	0.90	0.09	65,65,65,65	0
56	MG	1A	3051	1/1	0.90	0.13	26,26,26,26	0
56	MG	1A	3046	1/1	0.90	0.10	34,34,34,34	0
56	MG	1A	3336	1/1	0.90	0.34	52,52,52,52	0
56	MG	1A	3337	1/1	0.90	0.50	35,35,35,35	0
56	MG	2A	3310	1/1	0.90	0.14	80,80,80,80	0
56	MG	2A	3001	1/1	0.90	0.13	46,46,46,46	0
56	MG	1A	3749	1/1	0.90	0.16	37,37,37,37	0
56	MG	2A	3183	1/1	0.90	0.49	54,54,54,54	0
56	MG	2A	3315	1/1	0.90	0.20	49,49,49,49	0
56	MG	1x	111	1/1	0.90	0.17	62,62,62,62	0
56	MG	1a	1608	1/1	0.90	0.17	56,56,56,56	0
56	MG	1a	1609	1/1	0.90	0.11	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	3215	1/1	0.90	0.74	44,44,44,44	0
56	MG	2A	3791	1/1	0.90	0.06	67,67,67,67	0
56	MG	2A	3008	1/1	0.90	0.17	38,38,38,38	0
56	MG	1A	3414	1/1	0.90	0.13	44,44,44,44	0
56	MG	1A	3188	1/1	0.90	0.38	30,30,30,30	0
56	MG	2A	3018	1/1	0.90	0.18	60,60,60,60	0
56	MG	2B	206	1/1	0.90	0.14	76,76,76,76	0
56	MG	2B	208	1/1	0.90	0.27	64,64,64,64	0
56	MG	2A	3610	1/1	0.90	0.21	47,47,47,47	0
56	MG	1A	3623	1/1	0.90	0.14	26,26,26,26	0
56	MG	2A	3325	1/1	0.90	0.22	69,69,69,69	0
56	MG	1A	3473	1/1	0.90	0.32	34,34,34,34	0
56	MG	1A	3627	1/1	0.90	0.13	29,29,29,29	0
56	MG	2A	3447	1/1	0.90	0.42	71,71,71,71	0
56	MG	1A	3292	1/1	0.90	0.25	50,50,50,50	0
56	MG	1a	1642	1/1	0.90	0.24	58,58,58,58	0
56	MG	2a	1785	1/1	0.90	0.17	53,53,53,53	0
56	MG	2a	1789	1/1	0.90	0.13	45,45,45,45	0
56	MG	1A	3171	1/1	0.90	0.46	41,41,41,41	0
56	MG	1A	3773	1/1	0.90	0.05	58,58,58,58	0
56	MG	2E	305	1/1	0.90	0.32	64,64,64,64	0
56	MG	2a	1795	1/1	0.90	0.17	70,70,70,70	0
56	MG	1A	3909	1/1	0.90	0.49	78,78,78,78	0
56	MG	1A	3775	1/1	0.90	0.22	35,35,35,35	0
56	MG	2a	1798	1/1	0.90	0.14	62,62,62,62	0
56	MG	2A	3633	1/1	0.90	0.11	63,63,63,63	0
56	MG	1A	3779	1/1	0.90	0.20	80,80,80,80	0
56	MG	1A	3912	1/1	0.90	0.14	49,49,49,49	0
56	MG	1A	3785	1/1	0.90	0.14	17,17,17,17	0
56	MG	1A	3120	1/1	0.90	0.50	47,47,47,47	0
56	MG	2a	1806	1/1	0.90	0.15	76,76,76,76	0
56	MG	1A	3422	1/1	0.90	0.28	35,35,35,35	0
56	MG	2A	3644	1/1	0.90	0.18	53,53,53,53	0
56	MG	2A	3651	1/1	0.90	0.21	48,48,48,48	0
56	MG	2T	201	1/1	0.90	0.38	58,58,58,58	0
56	MG	1A	3251	1/1	0.90	0.14	60,60,60,60	0
56	MG	2T	203	1/1	0.90	0.13	52,52,52,52	0
56	MG	2A	3347	1/1	0.90	0.11	64,64,64,64	0
56	MG	2A	3231	1/1	0.90	0.43	60,60,60,60	0
56	MG	1A	3274	1/1	0.90	0.66	37,37,37,37	0
56	MG	2A	3663	1/1	0.90	0.21	34,34,34,34	0
56	MG	1A	3484	1/1	0.90	0.17	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3352	1/1	0.90	0.28	39,39,39,39	0
56	MG	1a	1698	1/1	0.90	0.17	42,42,42,42	0
56	MG	1a	1702	1/1	0.90	0.24	56,56,56,56	0
56	MG	2a	1602	1/1	0.90	0.18	62,62,62,62	0
56	MG	1a	1705	1/1	0.90	0.16	63,63,63,63	0
56	MG	2d	301	1/1	0.90	0.22	43,43,43,43	0
56	MG	1A	3555	1/1	0.90	0.45	41,41,41,41	0
56	MG	2A	3481	1/1	0.90	0.11	65,65,65,65	0
56	MG	2g	201	1/1	0.90	0.20	62,62,62,62	0
56	MG	1A	3929	1/1	0.90	0.13	37,37,37,37	0
56	MG	1a	1715	1/1	0.90	0.38	66,66,66,66	0
56	MG	1A	3658	1/1	0.90	0.16	35,35,35,35	0
56	MG	1A	3252	1/1	0.90	0.37	33,33,33,33	0
56	MG	1A	3179	1/1	0.90	0.10	44,44,44,44	0
56	MG	1a	1726	1/1	0.90	0.17	62,62,62,62	0
56	MG	1a	1731	1/1	0.90	0.12	60,60,60,60	0
56	MG	2A	3360	1/1	0.90	0.41	51,51,51,51	0
56	MG	1A	3813	1/1	0.90	0.11	27,27,27,27	0
56	MG	2A	3104	1/1	0.90	0.17	51,51,51,51	0
56	MG	1A	3138	1/1	0.90	0.48	28,28,28,28	0
56	MG	1A	4053	1/1	0.90	0.20	41,41,41,41	0
56	MG	1A	3666	1/1	0.90	0.13	22,22,22,22	0
56	MG	1a	1745	1/1	0.90	0.12	35,35,35,35	0
56	MG	1A	3309	1/1	0.90	0.27	48,48,48,48	0
56	MG	2A	3368	1/1	0.90	0.19	74,74,74,74	0
56	MG	2A	3705	1/1	0.90	0.13	69,69,69,69	0
56	MG	2a	1609	1/1	0.91	0.17	76,76,76,76	0
56	MG	1A	3768	1/1	0.91	0.15	20,20,20,20	0
56	MG	2A	3259	1/1	0.91	0.25	61,61,61,61	0
56	MG	1A	3449	1/1	0.91	0.56	51,51,51,51	0
56	MG	2A	3602	1/1	0.91	0.09	35,35,35,35	0
56	MG	1A	3170	1/1	0.91	0.15	43,43,43,43	0
56	MG	2a	1618	1/1	0.91	0.41	72,72,72,72	0
56	MG	2a	1619	1/1	0.91	0.12	76,76,76,76	0
56	MG	1a	1694	1/1	0.91	0.16	59,59,59,59	0
56	MG	1a	1695	1/1	0.91	0.23	43,43,43,43	0
56	MG	1A	3898	1/1	0.91	0.10	63,63,63,63	0
56	MG	1A	3772	1/1	0.91	0.13	17,17,17,17	0
56	MG	1A	3219	1/1	0.91	0.32	48,48,48,48	0
56	MG	1A	3654	1/1	0.91	0.16	24,24,24,24	0
56	MG	2A	3068	1/1	0.91	0.27	51,51,51,51	0
56	MG	1A	3496	1/1	0.91	0.08	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	3016	1/1	0.91	0.16	50,50,50,50	0
56	MG	2A	3416	1/1	0.91	0.11	58,58,58,58	0
56	MG	2A	3833	1/1	0.91	0.15	38,38,38,38	0
56	MG	1A	3411	1/1	0.91	0.60	44,44,44,44	0
56	MG	1a	1723	1/1	0.91	0.19	60,60,60,60	0
56	MG	2A	3076	1/1	0.91	0.13	40,40,40,40	0
56	MG	1A	4025	1/1	0.91	0.06	42,42,42,42	0
56	MG	1a	1734	1/1	0.91	0.10	54,54,54,54	0
56	MG	1A	3662	1/1	0.91	0.17	21,21,21,21	0
56	MG	1A	3261	1/1	0.91	0.53	40,40,40,40	0
56	MG	1A	3344	1/1	0.91	0.51	48,48,48,48	0
56	MG	1A	3796	1/1	0.91	0.46	30,30,30,30	0
56	MG	2A	3843	1/1	0.91	0.22	46,46,46,46	0
56	MG	1A	4032	1/1	0.91	0.09	47,47,47,47	0
56	MG	1A	3264	1/1	0.91	0.16	56,56,56,56	0
56	MG	1A	3464	1/1	0.91	0.16	65,65,65,65	0
56	MG	2A	3857	1/1	0.91	0.16	50,50,50,50	0
56	MG	1a	1748	1/1	0.91	0.14	62,62,62,62	0
56	MG	1A	4038	1/1	0.91	0.10	40,40,40,40	0
56	MG	2A	3116	1/1	0.91	0.28	70,70,70,70	0
56	MG	1a	1751	1/1	0.91	0.15	55,55,55,55	0
56	MG	2A	3646	1/1	0.91	0.13	42,42,42,42	0
56	MG	2a	1666	1/1	0.91	0.11	60,60,60,60	0
56	MG	2A	3647	1/1	0.91	0.18	60,60,60,60	0
56	MG	2A	3649	1/1	0.91	0.15	33,33,33,33	0
56	MG	2A	3286	1/1	0.91	0.13	46,46,46,46	0
56	MG	1a	1763	1/1	0.91	0.16	38,38,38,38	0
56	MG	2A	3440	1/1	0.91	0.18	50,50,50,50	0
56	MG	1A	3512	1/1	0.91	0.46	52,52,52,52	0
56	MG	1A	3579	1/1	0.91	0.34	59,59,59,59	0
56	MG	1a	1769	1/1	0.91	0.08	74,74,74,74	0
56	MG	2A	3443	1/1	0.91	0.25	48,48,48,48	0
56	MG	1A	4042	1/1	0.91	0.09	41,41,41,41	0
56	MG	1A	3674	1/1	0.91	0.09	64,64,64,64	0
56	MG	1A	3809	1/1	0.91	0.13	23,23,23,23	0
56	MG	2A	3673	1/1	0.91	0.09	71,71,71,71	0
56	MG	1A	3513	1/1	0.91	0.39	49,49,49,49	0
56	MG	1A	3933	1/1	0.91	0.25	37,37,37,37	0
56	MG	1A	3935	1/1	0.91	0.12	45,45,45,45	0
56	MG	2a	1699	1/1	0.91	0.21	65,65,65,65	0
56	MG	1A	3812	1/1	0.91	0.10	25,25,25,25	0
56	MG	2A	3682	1/1	0.91	0.14	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	4059	1/1	0.91	0.11	48,48,48,48	0
56	MG	2A	3307	1/1	0.91	0.11	59,59,59,59	0
56	MG	1A	3582	1/1	0.91	0.14	63,63,63,63	0
56	MG	2A	3458	1/1	0.91	0.64	58,58,58,58	0
56	MG	2a	1711	1/1	0.91	0.19	76,76,76,76	0
56	MG	2a	1712	1/1	0.91	0.23	68,68,68,68	0
56	MG	2A	3689	1/1	0.91	0.23	59,59,59,59	0
56	MG	1a	1793	1/1	0.91	0.09	51,51,51,51	0
56	MG	2a	1715	1/1	0.91	0.13	46,46,46,46	0
56	MG	2a	1716	1/1	0.91	0.17	70,70,70,70	0
56	MG	1A	3175	1/1	0.91	0.13	37,37,37,37	0
56	MG	1E	302	1/1	0.91	1.12	36,36,36,36	0
56	MG	1A	3819	1/1	0.91	0.10	49,49,49,49	0
56	MG	1A	3941	1/1	0.91	0.15	49,49,49,49	0
56	MG	2A	3140	1/1	0.91	0.58	41,41,41,41	0
56	MG	1F	305	1/1	0.91	0.09	43,43,43,43	0
56	MG	1A	4067	1/1	0.91	0.20	83,83,83,83	0
56	MG	2A	3143	1/1	0.91	0.15	57,57,57,57	0
56	MG	2A	3703	1/1	0.91	0.11	57,57,57,57	0
56	MG	1A	3198	1/1	0.91	0.14	21,21,21,21	0
56	MG	1A	4069	1/1	0.91	0.32	30,30,30,30	0
56	MG	2A	3709	1/1	0.91	0.09	52,52,52,52	0
56	MG	1A	3201	1/1	0.91	0.13	35,35,35,35	0
56	MG	1a	1821	1/1	0.91	0.05	87,87,87,87	0
56	MG	1A	3148	1/1	0.91	0.47	27,27,27,27	0
56	MG	2A	3713	1/1	0.91	0.12	40,40,40,40	0
56	MG	2a	1738	1/1	0.91	0.11	65,65,65,65	0
56	MG	1a	1824	1/1	0.91	0.17	51,51,51,51	0
56	MG	2A	3322	1/1	0.91	0.12	59,59,59,59	0
56	MG	1N	208	1/1	0.91	0.43	37,37,37,37	0
56	MG	1A	3420	1/1	0.91	0.17	49,49,49,49	0
56	MG	1A	3688	1/1	0.91	0.09	35,35,35,35	0
56	MG	1A	3384	1/1	0.91	0.24	41,41,41,41	0
56	MG	1Q	204	1/1	0.91	0.21	52,52,52,52	0
56	MG	1A	3954	1/1	0.91	0.23	35,35,35,35	0
56	MG	1A	3423	1/1	0.91	0.14	47,47,47,47	0
56	MG	1A	3203	1/1	0.91	0.17	26,26,26,26	0
56	MG	2A	3492	1/1	0.91	0.26	49,49,49,49	0
56	MG	1A	3831	1/1	0.91	0.12	34,34,34,34	0
56	MG	1d	3101	1/1	0.91	0.22	54,54,54,54	0
56	MG	1A	3272	1/1	0.91	0.17	54,54,54,54	0
56	MG	1A	3151	1/1	0.91	0.60	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3334	1/1	0.91	0.12	52,52,52,52	0
56	MG	1A	3835	1/1	0.91	0.09	53,53,53,53	0
56	MG	1p	101	1/1	0.91	0.20	44,44,44,44	0
56	MG	1A	3704	1/1	0.91	0.15	51,51,51,51	0
56	MG	1A	3534	1/1	0.91	0.25	34,34,34,34	0
56	MG	2a	1767	1/1	0.91	0.25	61,61,61,61	0
56	MG	1A	3706	1/1	0.91	0.20	53,53,53,53	0
56	MG	1A	4122	1/1	0.91	0.23	35,35,35,35	0
56	MG	1A	3967	1/1	0.91	0.30	66,66,66,66	0
56	MG	1A	3320	1/1	0.91	0.27	51,51,51,51	0
56	MG	1A	3536	1/1	0.91	0.12	56,56,56,56	0
56	MG	1A	3611	1/1	0.91	0.13	21,21,21,21	0
56	MG	1x	109	1/1	0.91	0.32	65,65,65,65	0
56	MG	1A	3851	1/1	0.91	0.09	51,51,51,51	0
56	MG	1A	3431	1/1	0.91	0.71	57,57,57,57	0
56	MG	15	102	1/1	0.91	0.62	38,38,38,38	0
56	MG	1A	3854	1/1	0.91	0.30	57,57,57,57	0
56	MG	1A	3856	1/1	0.91	0.15	41,41,41,41	0
56	MG	2A	3197	1/1	0.91	0.36	40,40,40,40	0
56	MG	2A	3518	1/1	0.91	0.52	61,61,61,61	0
56	MG	2A	3198	1/1	0.91	0.12	53,53,53,53	0
56	MG	1A	3857	1/1	0.91	0.24	54,54,54,54	0
56	MG	1A	3616	1/1	0.91	0.14	61,61,61,61	0
56	MG	2B	207	1/1	0.91	0.18	69,69,69,69	0
56	MG	1A	3980	1/1	0.91	0.13	52,52,52,52	0
56	MG	1A	3281	1/1	0.91	0.43	46,46,46,46	0
56	MG	1A	3181	1/1	0.91	0.19	51,51,51,51	0
56	MG	2A	3218	1/1	0.91	0.22	57,57,57,57	0
56	MG	2A	3007	1/1	0.91	0.21	64,64,64,64	0
56	MG	1a	1617	1/1	0.91	0.07	58,58,58,58	0
56	MG	1A	3742	1/1	0.91	0.14	40,40,40,40	0
56	MG	1a	1621	1/1	0.91	0.40	64,64,64,64	0
56	MG	2a	1813	1/1	0.91	0.10	74,74,74,74	0
56	MG	2A	3770	1/1	0.91	0.09	69,69,69,69	0
56	MG	1A	3987	1/1	0.91	0.41	47,47,47,47	0
56	MG	1A	3869	1/1	0.91	0.12	61,61,61,61	0
56	MG	2E	304	1/1	0.91	0.23	58,58,58,58	0
56	MG	1A	3992	1/1	0.91	0.06	70,70,70,70	0
56	MG	1A	3541	1/1	0.91	0.12	53,53,53,53	0
56	MG	2A	3020	1/1	0.91	0.15	54,54,54,54	0
56	MG	1A	3994	1/1	0.91	0.11	33,33,33,33	0
56	MG	2A	3024	1/1	0.91	0.12	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	1A	3871	1/1	0.91	0.10	46,46,46,46	0
56	MG	2a	1827	1/1	0.91	0.14	68,68,68,68	0
56	MG	2A	3786	1/1	0.91	0.11	49,49,49,49	0
56	MG	2P	203	1/1	0.91	0.14	49,49,49,49	0
56	MG	1A	3211	1/1	0.91	0.17	56,56,56,56	0
56	MG	2A	3029	1/1	0.91	0.23	56,56,56,56	0
56	MG	2f	201	1/1	0.91	0.17	51,51,51,51	0
56	MG	1a	1644	1/1	0.91	0.18	60,60,60,60	0
56	MG	1A	3754	1/1	0.91	0.42	45,45,45,45	0
56	MG	2A	3242	1/1	0.91	0.22	71,71,71,71	0
56	MG	2A	3244	1/1	0.91	0.17	41,41,41,41	0
56	MG	2A	3246	1/1	0.91	0.27	75,75,75,75	0
56	MG	2A	3389	1/1	0.91	0.17	69,69,69,69	0
56	MG	2A	3249	1/1	0.91	0.11	64,64,64,64	0
56	MG	2A	3798	1/1	0.91	0.11	82,82,82,82	0
56	MG	1A	3250	1/1	0.91	0.61	52,52,52,52	0
56	MG	2v	103	1/1	0.91	0.12	78,78,78,78	0
56	MG	1A	3039	1/1	0.91	0.45	38,38,38,38	0
56	MG	1A	3004	1/1	0.91	0.15	24,24,24,24	0
56	MG	1A	3075	1/1	0.91	0.13	28,28,28,28	0
56	MG	27	101	1/1	0.91	0.21	50,50,50,50	0
56	MG	1A	3550	1/1	0.91	0.17	51,51,51,51	0
56	MG	2y	104	1/1	0.91	0.21	52,52,52,52	0
56	MG	2A	3044	1/1	0.91	0.12	74,74,74,74	0
56	MG	2a	1603	1/1	0.91	0.15	63,63,63,63	0
56	MG	1a	1675	1/1	0.91	0.38	63,63,63,63	0
56	MG	1a	1683	1/1	0.91	0.14	54,54,54,54	0
56	MG	2A	3047	1/1	0.91	0.28	31,31,31,31	0
59	ZN	2n	501	1/1	0.91	0.09	97,97,97,97	0
56	MG	1A	4039	1/1	0.92	0.14	19,19,19,19	0
56	MG	2A	3303	1/1	0.92	0.17	55,55,55,55	0
56	MG	1A	3047	1/1	0.92	0.14	31,31,31,31	0
56	MG	1A	3330	1/1	0.92	0.17	46,46,46,46	0
56	MG	2U	202	1/1	0.92	0.16	50,50,50,50	0
56	MG	2U	204	1/1	0.92	0.56	57,57,57,57	0
56	MG	2A	3749	1/1	0.92	0.12	55,55,55,55	0
56	MG	2A	3118	1/1	0.92	0.13	56,56,56,56	0
56	MG	1A	3432	1/1	0.92	0.29	52,52,52,52	0
56	MG	1A	3667	1/1	0.92	0.13	18,18,18,18	0
56	MG	23	101	1/1	0.92	1.12	66,66,66,66	0
56	MG	1a	1633	1/1	0.92	0.09	41,41,41,41	0
56	MG	1A	4045	1/1	0.92	0.11	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3121	1/1	0.92	0.17	31,31,31,31	0
56	MG	1A	3932	1/1	0.92	0.13	38,38,38,38	0
56	MG	2a	1601	1/1	0.92	0.11	57,57,57,57	0
56	MG	2A	3125	1/1	0.92	0.19	60,60,60,60	0
56	MG	1a	1640	1/1	0.92	0.19	66,66,66,66	0
56	MG	1A	3218	1/1	0.92	0.71	57,57,57,57	0
56	MG	2A	3316	1/1	0.92	0.29	66,66,66,66	0
56	MG	2A	3761	1/1	0.92	0.12	63,63,63,63	0
56	MG	1A	3934	1/1	0.92	0.15	33,33,33,33	0
56	MG	1A	4054	1/1	0.92	0.15	25,25,25,25	0
56	MG	1A	3808	1/1	0.92	0.26	57,57,57,57	0
56	MG	1A	4056	1/1	0.92	0.18	48,48,48,48	0
56	MG	2A	3506	1/1	0.92	0.14	77,77,77,77	0
56	MG	1A	3671	1/1	0.92	0.15	18,18,18,18	0
56	MG	1A	4060	1/1	0.92	0.15	46,46,46,46	0
56	MG	1A	3570	1/1	0.92	0.25	44,44,44,44	0
56	MG	1a	1666	1/1	0.92	0.12	65,65,65,65	0
56	MG	2A	3511	1/1	0.92	0.52	42,42,42,42	0
56	MG	1A	3123	1/1	0.92	0.23	42,42,42,42	0
56	MG	1a	1669	1/1	0.92	0.09	52,52,52,52	0
56	MG	1A	3437	1/1	0.92	0.76	54,54,54,54	0
56	MG	1A	3814	1/1	0.92	0.22	58,58,58,58	0
56	MG	1a	1673	1/1	0.92	0.09	49,49,49,49	0
56	MG	2A	3779	1/1	0.92	0.12	36,36,36,36	0
56	MG	1a	1677	1/1	0.92	0.27	44,44,44,44	0
56	MG	1A	4066	1/1	0.92	0.20	30,30,30,30	0
56	MG	1a	1684	1/1	0.92	0.24	67,67,67,67	0
56	MG	1A	3440	1/1	0.92	0.43	42,42,42,42	0
56	MG	1A	3578	1/1	0.92	0.48	28,28,28,28	0
56	MG	2A	3331	1/1	0.92	0.10	66,66,66,66	0
56	MG	2A	3146	1/1	0.92	0.18	52,52,52,52	0
56	MG	1A	3220	1/1	0.92	0.58	48,48,48,48	0
56	MG	1A	3946	1/1	0.92	0.12	47,47,47,47	0
56	MG	1A	4079	1/1	0.92	0.21	69,69,69,69	0
56	MG	1A	3338	1/1	0.92	0.20	34,34,34,34	0
56	MG	1A	3508	1/1	0.92	0.60	35,35,35,35	0
56	MG	2A	3530	1/1	0.92	0.16	55,55,55,55	0
56	MG	1A	3509	1/1	0.92	0.69	34,34,34,34	0
56	MG	1A	3952	1/1	0.92	0.10	41,41,41,41	0
56	MG	2a	1654	1/1	0.92	0.09	79,79,79,79	0
56	MG	1A	3685	1/1	0.92	0.08	66,66,66,66	0
56	MG	1A	3444	1/1	0.92	0.32	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3275	1/1	0.92	0.39	38,38,38,38	0
56	MG	2A	3168	1/1	0.92	0.08	51,51,51,51	0
56	MG	1a	1718	1/1	0.92	0.23	56,56,56,56	0
56	MG	2A	3169	1/1	0.92	0.76	53,53,53,53	0
56	MG	2A	3804	1/1	0.92	0.30	70,70,70,70	0
56	MG	2A	3548	1/1	0.92	0.10	42,42,42,42	0
56	MG	2A	3170	1/1	0.92	0.15	43,43,43,43	0
56	MG	1A	3010	1/1	0.92	0.16	38,38,38,38	0
56	MG	2A	3809	1/1	0.92	0.16	57,57,57,57	0
56	MG	2A	3354	1/1	0.92	0.57	60,60,60,60	0
56	MG	1A	3591	1/1	0.92	0.34	31,31,31,31	0
56	MG	1A	3129	1/1	0.92	0.21	60,60,60,60	0
56	MG	1A	3699	1/1	0.92	0.13	33,33,33,33	0
56	MG	1A	4109	1/1	0.92	0.12	37,37,37,37	0
56	MG	2a	1684	1/1	0.92	0.08	52,52,52,52	0
56	MG	1A	3001	1/1	0.92	0.11	34,34,34,34	0
56	MG	2A	3571	1/1	0.92	0.15	36,36,36,36	0
56	MG	1A	3007	1/1	0.92	0.33	37,37,37,37	0
56	MG	1A	3965	1/1	0.92	0.21	52,52,52,52	0
56	MG	2A	3190	1/1	0.92	0.21	43,43,43,43	0
56	MG	2A	3579	1/1	0.92	0.15	32,32,32,32	0
56	MG	2A	3831	1/1	0.92	0.17	29,29,29,29	0
56	MG	1A	3596	1/1	0.92	0.16	37,37,37,37	0
56	MG	1A	3842	1/1	0.92	0.18	70,70,70,70	0
56	MG	1A	3396	1/1	0.92	0.64	36,36,36,36	0
56	MG	1A	3708	1/1	0.92	0.10	56,56,56,56	0
56	MG	1a	1759	1/1	0.92	0.12	39,39,39,39	0
56	MG	2A	3589	1/1	0.92	0.10	62,62,62,62	0
56	MG	1a	1761	1/1	0.92	0.25	60,60,60,60	0
56	MG	1A	4129	1/1	0.92	0.72	41,41,41,41	0
56	MG	1A	3971	1/1	0.92	0.17	28,28,28,28	0
56	MG	2A	3595	1/1	0.92	0.14	28,28,28,28	0
56	MG	2A	3373	1/1	0.92	1.12	65,65,65,65	0
56	MG	1A	3057	1/1	0.92	0.12	46,46,46,46	0
56	MG	1a	1770	1/1	0.92	0.10	93,93,93,93	0
56	MG	1A	3602	1/1	0.92	0.15	32,32,32,32	0
56	MG	2A	3849	1/1	0.92	0.84	49,49,49,49	0
56	MG	2A	3378	1/1	0.92	0.53	68,68,68,68	0
56	MG	2A	3199	1/1	0.92	0.20	61,61,61,61	0
56	MG	2A	3201	1/1	0.92	0.65	43,43,43,43	0
56	MG	1A	4144	1/1	0.92	0.15	46,46,46,46	0
56	MG	1a	1778	1/1	0.92	0.11	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	3609	1/1	0.92	0.16	46,46,46,46	0
56	MG	2a	1726	1/1	0.92	0.17	51,51,51,51	0
56	MG	2A	3862	1/1	0.92	0.10	52,52,52,52	0
56	MG	1B	201	1/1	0.92	0.34	53,53,53,53	0
56	MG	1A	3974	1/1	0.92	0.11	37,37,37,37	0
56	MG	1A	3849	1/1	0.92	0.62	48,48,48,48	0
56	MG	1B	208	1/1	0.92	0.18	56,56,56,56	0
56	MG	1A	3059	1/1	0.92	0.21	48,48,48,48	0
56	MG	1A	3715	1/1	0.92	0.12	35,35,35,35	0
56	MG	2A	3217	1/1	0.92	0.42	62,62,62,62	0
56	MG	1A	3853	1/1	0.92	0.12	45,45,45,45	0
56	MG	2A	3002	1/1	0.92	0.11	57,57,57,57	0
56	MG	1A	3190	1/1	0.92	0.12	44,44,44,44	0
56	MG	2A	3223	1/1	0.92	0.43	60,60,60,60	0
56	MG	1a	1800	1/1	0.92	0.19	74,74,74,74	0
56	MG	1A	3855	1/1	0.92	0.14	34,34,34,34	0
56	MG	2A	3631	1/1	0.92	0.17	53,53,53,53	0
56	MG	1B	226	1/1	0.92	0.10	60,60,60,60	0
56	MG	1A	3351	1/1	0.92	0.38	53,53,53,53	0
56	MG	1A	3735	1/1	0.92	0.08	20,20,20,20	0
56	MG	1A	3238	1/1	0.92	0.09	43,43,43,43	0
56	MG	2A	3010	1/1	0.92	0.17	62,62,62,62	0
56	MG	2A	3014	1/1	0.92	0.14	50,50,50,50	0
56	MG	1A	3240	1/1	0.92	0.65	41,41,41,41	0
56	MG	2A	3403	1/1	0.92	0.37	45,45,45,45	0
56	MG	1a	1818	1/1	0.92	0.13	53,53,53,53	0
56	MG	1A	3988	1/1	0.92	0.17	23,23,23,23	0
56	MG	1A	3063	1/1	0.92	0.18	55,55,55,55	0
56	MG	1A	3044	1/1	0.92	0.71	38,38,38,38	0
56	MG	1D	310	1/1	0.92	0.58	47,47,47,47	0
56	MG	1a	1825	1/1	0.92	0.08	74,74,74,74	0
56	MG	2A	3021	1/1	0.92	0.24	48,48,48,48	0
56	MG	1A	3618	1/1	0.92	0.16	29,29,29,29	0
56	MG	2a	1768	1/1	0.92	0.10	60,60,60,60	0
56	MG	1A	3248	1/1	0.92	0.13	41,41,41,41	0
56	MG	2A	3025	1/1	0.92	0.20	57,57,57,57	0
56	MG	1a	1832	1/1	0.92	0.18	66,66,66,66	0
56	MG	2A	3248	1/1	0.92	0.31	69,69,69,69	0
56	MG	1A	3995	1/1	0.92	0.17	18,18,18,18	0
56	MG	2a	1778	1/1	0.92	0.16	67,67,67,67	0
56	MG	1A	3296	1/1	0.92	0.35	29,29,29,29	0
56	MG	2A	3665	1/1	0.92	0.23	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3197	1/1	0.92	0.17	37,37,37,37	0
56	MG	1a	1842	1/1	0.92	0.90	58,58,58,58	0
56	MG	2A	3669	1/1	0.92	0.10	55,55,55,55	0
56	MG	1A	3538	1/1	0.92	0.23	39,39,39,39	0
56	MG	1A	3762	1/1	0.92	0.44	29,29,29,29	0
56	MG	2A	3420	1/1	0.92	0.96	55,55,55,55	0
56	MG	2A	3036	1/1	0.92	0.10	40,40,40,40	0
56	MG	1A	3096	1/1	0.92	0.20	54,54,54,54	0
56	MG	1m	201	1/1	0.92	0.15	42,42,42,42	0
56	MG	1A	3476	1/1	0.92	0.33	38,38,38,38	0
56	MG	1A	3767	1/1	0.92	0.11	21,21,21,21	0
56	MG	1A	3150	1/1	0.92	0.65	34,34,34,34	0
56	MG	2A	3427	1/1	0.92	0.11	64,64,64,64	0
56	MG	1A	3769	1/1	0.92	0.11	36,36,36,36	0
56	MG	2A	3045	1/1	0.92	0.23	64,64,64,64	0
56	MG	1w	102	1/1	0.92	0.11	63,63,63,63	0
56	MG	1A	3890	1/1	0.92	0.12	43,43,43,43	0
56	MG	2a	1809	1/1	0.92	0.19	66,66,66,66	0
56	MG	1Q	205	1/1	0.92	0.13	44,44,44,44	0
56	MG	2A	3264	1/1	0.92	0.19	66,66,66,66	0
56	MG	1S	203	1/1	0.92	0.37	67,67,67,67	0
56	MG	1T	201	1/1	0.92	0.10	54,54,54,54	0
56	MG	2A	3051	1/1	0.92	0.14	73,73,73,73	0
56	MG	1A	4012	1/1	0.92	0.13	84,84,84,84	0
56	MG	2A	3698	1/1	0.92	0.20	52,52,52,52	0
56	MG	1A	3638	1/1	0.92	0.25	69,69,69,69	0
56	MG	2A	3700	1/1	0.92	0.13	65,65,65,65	0
56	MG	1A	3101	1/1	0.92	0.17	62,62,62,62	0
56	MG	1A	3153	1/1	0.92	0.27	42,42,42,42	0
56	MG	1A	3205	1/1	0.92	0.47	46,46,46,46	0
56	MG	1A	3900	1/1	0.92	0.85	36,36,36,36	0
56	MG	1A	3158	1/1	0.92	0.49	27,27,27,27	0
56	MG	2A	3708	1/1	0.92	0.12	59,59,59,59	0
56	MG	2a	1830	1/1	0.92	0.29	60,60,60,60	0
56	MG	1A	3071	1/1	0.92	0.64	31,31,31,31	0
56	MG	1A	3781	1/1	0.92	0.18	42,42,42,42	0
56	MG	2d	302	1/1	0.92	0.10	57,57,57,57	0
56	MG	1A	3907	1/1	0.92	0.11	67,67,67,67	0
56	MG	1A	3782	1/1	0.92	0.18	59,59,59,59	0
56	MG	1A	3113	1/1	0.92	0.14	31,31,31,31	0
56	MG	2A	3081	1/1	0.92	0.27	41,41,41,41	0
56	MG	2A	3085	1/1	0.92	0.19	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	1A	3018	1/1	0.92	0.15	24,24,24,24	0
56	MG	2A	3090	1/1	0.92	0.14	49,49,49,49	0
56	MG	2A	3091	1/1	0.92	0.68	44,44,44,44	0
56	MG	2A	3727	1/1	0.92	0.11	56,56,56,56	0
56	MG	2D	303	1/1	0.92	0.15	67,67,67,67	0
56	MG	2r	101	1/1	0.92	0.34	66,66,66,66	0
56	MG	2E	301	1/1	0.92	0.10	51,51,51,51	0
56	MG	2A	3093	1/1	0.92	1.13	52,52,52,52	0
56	MG	17	102	1/1	0.92	0.40	57,57,57,57	0
56	MG	1A	4030	1/1	0.92	0.37	53,53,53,53	0
56	MG	2A	3290	1/1	0.92	0.76	53,53,53,53	0
56	MG	2A	3101	1/1	0.92	0.36	57,57,57,57	0
56	MG	2y	101	1/1	0.92	0.20	61,61,61,61	0
56	MG	2y	102	1/1	0.92	0.12	76,76,76,76	0
56	MG	2A	3476	1/1	0.92	0.44	47,47,47,47	0
56	MG	1A	3789	1/1	0.92	0.08	53,53,53,53	0
56	MG	1A	3554	1/1	0.92	0.67	48,48,48,48	0
56	MG	1A	3117	1/1	0.92	0.66	41,41,41,41	0
56	MG	1a	1615	1/1	0.92	0.12	57,57,57,57	0
56	MG	1A	3373	1/1	0.92	0.74	46,46,46,46	0
59	ZN	14	501	1/1	0.92	0.13	94,94,94,94	0
59	ZN	2Y	201	1/1	0.92	0.08	106,106,106,106	0
56	MG	1A	3794	1/1	0.92	0.07	37,37,37,37	0
56	MG	2A	3300	1/1	0.92	0.45	63,63,63,63	0
56	MG	1a	1732	1/1	0.93	0.12	50,50,50,50	0
56	MG	2a	1622	1/1	0.93	0.36	72,72,72,72	0
56	MG	1A	3475	1/1	0.93	0.58	49,49,49,49	0
56	MG	2A	3012	1/1	0.93	0.24	36,36,36,36	0
56	MG	1A	3027	1/1	0.93	0.24	50,50,50,50	0
56	MG	2a	1626	1/1	0.93	0.28	64,64,64,64	0
56	MG	2A	3185	1/1	0.93	0.15	43,43,43,43	0
56	MG	2a	1628	1/1	0.93	0.43	65,65,65,65	0
56	MG	1A	3122	1/1	0.93	0.48	41,41,41,41	0
56	MG	2A	3016	1/1	0.93	0.17	53,53,53,53	0
56	MG	1A	3815	1/1	0.93	0.09	42,42,42,42	0
56	MG	1A	3204	1/1	0.93	0.09	49,49,49,49	0
56	MG	1B	224	1/1	0.93	0.12	59,59,59,59	0
56	MG	2A	3690	1/1	0.93	0.16	54,54,54,54	0
56	MG	1A	3921	1/1	0.93	0.06	47,47,47,47	0
56	MG	2A	3693	1/1	0.93	0.12	63,63,63,63	0
56	MG	1A	3922	1/1	0.93	0.12	20,20,20,20	0
56	MG	1A	3923	1/1	0.93	0.17	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	2A	3697	1/1	0.93	0.25	65,65,65,65	0
56	MG	1A	3426	1/1	0.93	0.09	58,58,58,58	0
56	MG	1A	3613	1/1	0.93	0.09	12,12,12,12	0
56	MG	1A	3102	1/1	0.93	0.32	41,41,41,41	0
56	MG	1A	3617	1/1	0.93	0.19	33,33,33,33	0
56	MG	1A	3233	1/1	0.93	0.12	65,65,65,65	0
56	MG	1A	3543	1/1	0.93	0.81	46,46,46,46	0
56	MG	1A	3303	1/1	0.93	0.18	40,40,40,40	0
56	MG	1A	3730	1/1	0.93	0.13	47,47,47,47	0
56	MG	2A	3707	1/1	0.93	0.18	44,44,44,44	0
56	MG	2a	1657	1/1	0.93	0.15	53,53,53,53	0
56	MG	2A	3212	1/1	0.93	0.12	35,35,35,35	0
56	MG	1A	3388	1/1	0.93	0.10	72,72,72,72	0
56	MG	1E	305	1/1	0.93	0.10	37,37,37,37	0
56	MG	1A	3734	1/1	0.93	0.14	31,31,31,31	0
56	MG	1F	301	1/1	0.93	0.07	31,31,31,31	0
56	MG	1A	3104	1/1	0.93	0.29	33,33,33,33	0
56	MG	2a	1664	1/1	0.93	0.09	62,62,62,62	0
56	MG	1A	3629	1/1	0.93	0.12	53,53,53,53	0
56	MG	1A	3350	1/1	0.93	0.09	59,59,59,59	0
56	MG	1A	3632	1/1	0.93	0.06	44,44,44,44	0
56	MG	1A	3748	1/1	0.93	0.15	20,20,20,20	0
56	MG	2A	3509	1/1	0.93	0.35	53,53,53,53	0
56	MG	2A	3050	1/1	0.93	0.14	56,56,56,56	0
56	MG	1A	3269	1/1	0.93	0.46	43,43,43,43	0
56	MG	2A	3226	1/1	0.93	0.13	47,47,47,47	0
56	MG	2A	3361	1/1	0.93	0.15	49,49,49,49	0
56	MG	1N	202	1/1	0.93	0.51	43,43,43,43	0
56	MG	1A	3029	1/1	0.93	0.49	39,39,39,39	0
56	MG	1A	4049	1/1	0.93	0.08	39,39,39,39	0
56	MG	1A	3948	1/1	0.93	0.09	32,32,32,32	0
56	MG	1A	3752	1/1	0.93	0.17	35,35,35,35	0
56	MG	1O	202	1/1	0.93	0.14	62,62,62,62	0
56	MG	1A	3353	1/1	0.93	0.16	55,55,55,55	0
56	MG	1A	3951	1/1	0.93	0.09	15,15,15,15	0
56	MG	1Q	203	1/1	0.93	0.26	57,57,57,57	0
56	MG	1A	3161	1/1	0.93	1.79	38,38,38,38	0
56	MG	1A	3557	1/1	0.93	0.12	19,19,19,19	0
56	MG	1R	201	1/1	0.93	0.15	51,51,51,51	0
56	MG	1a	1807	1/1	0.93	0.12	67,67,67,67	0
56	MG	1A	3850	1/1	0.93	0.12	54,54,54,54	0
56	MG	1S	201	1/1	0.93	1.01	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	3757	1/1	0.93	0.15	40,40,40,40	0
56	MG	1A	3759	1/1	0.93	0.13	27,27,27,27	0
56	MG	2A	3072	1/1	0.93	0.29	57,57,57,57	0
56	MG	2A	3245	1/1	0.93	0.06	59,59,59,59	0
56	MG	2A	3747	1/1	0.93	0.08	59,59,59,59	0
56	MG	2A	3074	1/1	0.93	0.22	60,60,60,60	0
56	MG	1A	3312	1/1	0.93	0.10	42,42,42,42	0
56	MG	1A	3443	1/1	0.93	0.20	48,48,48,48	0
56	MG	1X	102	1/1	0.93	0.64	39,39,39,39	0
56	MG	1A	3398	1/1	0.93	0.84	40,40,40,40	0
56	MG	1A	3107	1/1	0.93	0.20	28,28,28,28	0
56	MG	1A	3564	1/1	0.93	0.62	35,35,35,35	0
56	MG	1A	3859	1/1	0.93	0.29	28,28,28,28	0
56	MG	1a	1830	1/1	0.93	0.19	65,65,65,65	0
56	MG	1A	3246	1/1	0.93	0.65	42,42,42,42	0
56	MG	1A	4072	1/1	0.93	0.29	71,71,71,71	0
56	MG	2A	3096	1/1	0.93	0.15	55,55,55,55	0
56	MG	2a	1729	1/1	0.93	0.09	78,78,78,78	0
56	MG	2A	3556	1/1	0.93	0.12	33,33,33,33	0
56	MG	1A	3861	1/1	0.93	0.85	54,54,54,54	0
56	MG	2A	3762	1/1	0.93	0.20	69,69,69,69	0
56	MG	1A	3321	1/1	0.93	0.13	51,51,51,51	0
56	MG	2A	3564	1/1	0.93	0.13	57,57,57,57	0
56	MG	2a	1735	1/1	0.93	0.21	66,66,66,66	0
56	MG	1a	1843	1/1	0.93	0.07	52,52,52,52	0
56	MG	1A	3863	1/1	0.93	0.33	29,29,29,29	0
56	MG	2A	3766	1/1	0.93	0.27	64,64,64,64	0
56	MG	1A	3864	1/1	0.93	0.97	41,41,41,41	0
56	MG	2A	3569	1/1	0.93	0.15	47,47,47,47	0
56	MG	1A	3189	1/1	0.93	0.94	44,44,44,44	0
56	MG	1A	3867	1/1	0.93	0.77	38,38,38,38	0
56	MG	18	101	1/1	0.93	0.15	45,45,45,45	0
56	MG	2A	3572	1/1	0.93	0.13	36,36,36,36	0
56	MG	1m	203	1/1	0.93	0.18	49,49,49,49	0
56	MG	1a	1602	1/1	0.93	0.13	42,42,42,42	0
56	MG	2a	1749	1/1	0.93	0.04	85,85,85,85	0
56	MG	2A	3573	1/1	0.93	0.14	46,46,46,46	0
56	MG	2a	1753	1/1	0.93	0.12	67,67,67,67	0
56	MG	1s	3701	1/1	0.93	0.20	61,61,61,61	0
56	MG	2A	3110	1/1	0.93	0.17	70,70,70,70	0
56	MG	1A	4090	1/1	0.93	0.11	61,61,61,61	0
56	MG	1A	3093	1/1	0.93	0.11	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	3777	1/1	0.93	0.10	66,66,66,66	0
56	MG	1w	105	1/1	0.93	0.09	64,64,64,64	0
56	MG	1A	3324	1/1	0.93	0.15	55,55,55,55	0
56	MG	1x	101	1/1	0.93	0.18	54,54,54,54	0
56	MG	1a	1613	1/1	0.93	0.11	68,68,68,68	0
56	MG	1x	104	1/1	0.93	0.21	67,67,67,67	0
56	MG	2A	3117	1/1	0.93	0.11	54,54,54,54	0
56	MG	2A	3782	1/1	0.93	0.18	67,67,67,67	0
56	MG	1A	4095	1/1	0.93	0.16	54,54,54,54	0
56	MG	1a	1618	1/1	0.93	0.11	45,45,45,45	0
56	MG	2A	3585	1/1	0.93	0.12	45,45,45,45	0
56	MG	1A	3574	1/1	0.93	0.45	33,33,33,33	0
56	MG	1A	3575	1/1	0.93	0.47	40,40,40,40	0
56	MG	1A	3777	1/1	0.93	0.12	46,46,46,46	0
56	MG	1A	4101	1/1	0.93	0.25	47,47,47,47	0
56	MG	2a	1779	1/1	0.93	0.14	79,79,79,79	0
56	MG	1a	1627	1/1	0.93	0.14	49,49,49,49	0
56	MG	2A	3277	1/1	0.93	0.40	58,58,58,58	0
56	MG	2A	3594	1/1	0.93	0.17	38,38,38,38	0
56	MG	2a	1788	1/1	0.93	0.12	60,60,60,60	0
56	MG	1A	4102	1/1	0.93	0.97	41,41,41,41	0
56	MG	1A	3455	1/1	0.93	0.10	49,49,49,49	0
56	MG	1A	3874	1/1	0.93	0.12	18,18,18,18	0
56	MG	1A	3249	1/1	0.93	0.19	51,51,51,51	0
56	MG	1A	3457	1/1	0.93	0.12	40,40,40,40	0
56	MG	1A	4113	1/1	0.93	0.11	49,49,49,49	0
56	MG	2A	3131	1/1	0.93	0.16	44,44,44,44	0
56	MG	1A	3363	1/1	0.93	0.68	61,61,61,61	0
56	MG	1A	4120	1/1	0.93	1.07	39,39,39,39	0
56	MG	1a	1643	1/1	0.93	0.16	60,60,60,60	0
56	MG	2A	3287	1/1	0.93	0.56	47,47,47,47	0
56	MG	2A	3424	1/1	0.93	0.14	69,69,69,69	0
56	MG	2A	3614	1/1	0.93	0.25	66,66,66,66	0
56	MG	1a	1648	1/1	0.93	0.12	42,42,42,42	0
56	MG	2A	3288	1/1	0.93	0.44	47,47,47,47	0
56	MG	2E	303	1/1	0.93	0.26	51,51,51,51	0
56	MG	1a	1656	1/1	0.93	0.28	54,54,54,54	0
56	MG	1A	3786	1/1	0.93	0.17	19,19,19,19	0
56	MG	1A	3787	1/1	0.93	0.20	36,36,36,36	0
56	MG	2E	308	1/1	0.93	0.13	65,65,65,65	0
56	MG	2A	3622	1/1	0.93	0.11	61,61,61,61	0
56	MG	1A	3461	1/1	0.93	0.24	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2F	303	1/1	0.93	0.36	49,49,49,49	0
56	MG	2a	1818	1/1	0.93	0.15	77,77,77,77	0
56	MG	1A	4126	1/1	0.93	1.00	41,41,41,41	0
56	MG	2G	201	1/1	0.93	0.11	62,62,62,62	0
56	MG	1A	3015	1/1	0.93	0.34	37,37,37,37	0
56	MG	1A	3517	1/1	0.93	0.15	58,58,58,58	0
56	MG	2A	3295	1/1	0.93	0.10	70,70,70,70	0
56	MG	1A	4135	1/1	0.93	0.32	42,42,42,42	0
56	MG	2A	3823	1/1	0.93	0.06	43,43,43,43	0
56	MG	1A	4139	1/1	0.93	0.67	35,35,35,35	0
56	MG	1A	3169	1/1	0.93	0.26	50,50,50,50	0
56	MG	2A	3149	1/1	0.93	0.39	58,58,58,58	0
56	MG	1A	3045	1/1	0.93	0.19	33,33,33,33	0
56	MG	1A	3119	1/1	0.93	0.97	39,39,39,39	0
56	MG	1A	3416	1/1	0.93	0.34	55,55,55,55	0
56	MG	1A	3903	1/1	0.93	0.23	20,20,20,20	0
56	MG	1A	4002	1/1	0.93	0.10	32,32,32,32	0
56	MG	1A	3524	1/1	0.93	0.22	37,37,37,37	0
56	MG	1A	3684	1/1	0.93	0.15	23,23,23,23	0
56	MG	1A	3335	1/1	0.93	0.26	46,46,46,46	0
56	MG	1A	3255	1/1	0.93	0.19	53,53,53,53	0
56	MG	21	101	1/1	0.93	0.11	62,62,62,62	0
56	MG	2A	3003	1/1	0.93	0.10	61,61,61,61	0
56	MG	1A	3199	1/1	0.93	0.10	35,35,35,35	0
56	MG	2A	3844	1/1	0.93	0.11	51,51,51,51	0
56	MG	1A	3807	1/1	0.93	0.11	41,41,41,41	0
56	MG	1a	1699	1/1	0.93	0.25	47,47,47,47	0
56	MG	2A	3006	1/1	0.93	0.17	62,62,62,62	0
56	MG	2A	3172	1/1	0.93	0.16	49,49,49,49	0
56	MG	2A	3851	1/1	0.93	0.51	73,73,73,73	0
56	MG	2A	3462	1/1	0.93	0.21	40,40,40,40	0
56	MG	1a	1711	1/1	0.93	0.16	39,39,39,39	0
56	MG	1A	3471	1/1	0.93	0.23	61,61,61,61	0
56	MG	2a	1607	1/1	0.93	0.17	64,64,64,64	0
56	MG	2a	1608	1/1	0.93	0.12	74,74,74,74	0
56	MG	1A	3100	1/1	0.93	0.20	52,52,52,52	0
56	MG	2A	3670	1/1	0.93	0.19	43,43,43,43	0
56	MG	2A	3468	1/1	0.93	0.28	41,41,41,41	0
56	MG	2a	1614	1/1	0.93	0.07	67,67,67,67	0
56	MG	2A	3672	1/1	0.93	0.06	46,46,46,46	0
56	MG	2A	3469	1/1	0.93	0.25	39,39,39,39	0
56	MG	2A	3471	1/1	0.93	0.22	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	1B	205	1/1	0.93	0.21	57,57,57,57	0
56	MG	1A	3258	1/1	0.93	0.20	52,52,52,52	0
56	MG	2A	3205	1/1	0.94	0.23	47,47,47,47	0
56	MG	2A	3033	1/1	0.94	0.33	54,54,54,54	0
56	MG	1a	1635	1/1	0.94	0.14	36,36,36,36	0
56	MG	2A	3208	1/1	0.94	0.14	70,70,70,70	0
56	MG	2A	3210	1/1	0.94	0.09	59,59,59,59	0
56	MG	2A	3560	1/1	0.94	0.15	54,54,54,54	0
56	MG	1a	1639	1/1	0.94	0.10	60,60,60,60	0
56	MG	1A	3304	1/1	0.94	0.18	39,39,39,39	0
56	MG	1A	3262	1/1	0.94	0.13	43,43,43,43	0
56	MG	2V	202	1/1	0.94	0.16	51,51,51,51	0
56	MG	2A	3370	1/1	0.94	0.31	59,59,59,59	0
56	MG	2A	3566	1/1	0.94	0.14	51,51,51,51	0
56	MG	2A	3567	1/1	0.94	0.14	48,48,48,48	0
56	MG	2A	3371	1/1	0.94	0.40	55,55,55,55	0
56	MG	1A	3451	1/1	0.94	0.16	57,57,57,57	0
56	MG	1a	1651	1/1	0.94	0.20	40,40,40,40	0
56	MG	1A	3452	1/1	0.94	0.21	40,40,40,40	0
56	MG	1A	3585	1/1	0.94	0.27	38,38,38,38	0
56	MG	2A	3793	1/1	0.94	0.09	63,63,63,63	0
56	MG	1A	3401	1/1	0.94	0.26	48,48,48,48	0
56	MG	1A	3402	1/1	0.94	0.15	43,43,43,43	0
56	MG	1A	3926	1/1	0.94	0.09	37,37,37,37	0
56	MG	2A	3222	1/1	0.94	0.30	63,63,63,63	0
56	MG	2A	3049	1/1	0.94	0.15	60,60,60,60	0
56	MG	1a	1665	1/1	0.94	0.11	65,65,65,65	0
56	MG	2A	3224	1/1	0.94	0.79	68,68,68,68	0
56	MG	2A	3580	1/1	0.94	0.13	37,37,37,37	0
56	MG	1A	3687	1/1	0.94	0.14	35,35,35,35	0
56	MG	1A	3589	1/1	0.94	0.22	32,32,32,32	0
56	MG	2a	1612	1/1	0.94	0.17	71,71,71,71	0
56	MG	1A	3130	1/1	0.94	0.07	35,35,35,35	0
56	MG	1A	3931	1/1	0.94	0.18	44,44,44,44	0
56	MG	1A	3060	1/1	0.94	0.12	41,41,41,41	0
56	MG	1a	1674	1/1	0.94	0.25	61,61,61,61	0
56	MG	2A	3588	1/1	0.94	0.18	71,71,71,71	0
56	MG	1A	3405	1/1	0.94	0.65	36,36,36,36	0
56	MG	1a	1680	1/1	0.94	0.26	48,48,48,48	0
56	MG	2A	3812	1/1	0.94	0.13	61,61,61,61	0
56	MG	2A	3813	1/1	0.94	0.13	56,56,56,56	0
56	MG	2A	3232	1/1	0.94	0.16	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	2A	3591	1/1	0.94	0.15	34,34,34,34	0
56	MG	2A	3816	1/1	0.94	0.12	28,28,28,28	0
56	MG	2A	3592	1/1	0.94	0.13	33,33,33,33	0
56	MG	1A	3091	1/1	0.94	0.22	51,51,51,51	0
56	MG	2A	3059	1/1	0.94	0.12	48,48,48,48	0
56	MG	2A	3061	1/1	0.94	0.33	48,48,48,48	0
56	MG	1A	3310	1/1	0.94	0.20	41,41,41,41	0
56	MG	2a	1631	1/1	0.94	0.21	50,50,50,50	0
56	MG	1a	1697	1/1	0.94	0.19	41,41,41,41	0
56	MG	2A	3598	1/1	0.94	0.15	29,29,29,29	0
56	MG	2A	3238	1/1	0.94	0.14	28,28,28,28	0
56	MG	2a	1639	1/1	0.94	0.15	63,63,63,63	0
56	MG	1a	1700	1/1	0.94	0.32	59,59,59,59	0
56	MG	2A	3063	1/1	0.94	0.13	48,48,48,48	0
56	MG	1A	3050	1/1	0.94	0.19	42,42,42,42	0
56	MG	2A	3830	1/1	0.94	0.20	46,46,46,46	0
56	MG	2A	3067	1/1	0.94	0.29	60,60,60,60	0
56	MG	1a	1710	1/1	0.94	0.14	70,70,70,70	0
56	MG	1A	3314	1/1	0.94	0.16	48,48,48,48	0
56	MG	1a	1712	1/1	0.94	0.43	52,52,52,52	0
56	MG	1A	3525	1/1	0.94	0.17	40,40,40,40	0
56	MG	1A	3410	1/1	0.94	0.88	44,44,44,44	0
56	MG	1a	1716	1/1	0.94	0.13	56,56,56,56	0
56	MG	2A	3835	1/1	0.94	0.05	73,73,73,73	0
56	MG	1A	3231	1/1	0.94	0.32	51,51,51,51	0
56	MG	1A	3319	1/1	0.94	0.12	55,55,55,55	0
56	MG	1a	1720	1/1	0.94	0.13	51,51,51,51	0
56	MG	2a	1656	1/1	0.94	0.39	71,71,71,71	0
56	MG	2A	3073	1/1	0.94	0.10	55,55,55,55	0
56	MG	1A	3232	1/1	0.94	0.49	44,44,44,44	0
56	MG	1A	4062	1/1	0.94	0.08	61,61,61,61	0
56	MG	1a	1728	1/1	0.94	0.17	55,55,55,55	0
56	MG	1A	3610	1/1	0.94	0.13	29,29,29,29	0
56	MG	2A	3084	1/1	0.94	0.13	48,48,48,48	0
56	MG	1a	1733	1/1	0.94	0.10	52,52,52,52	0
56	MG	2A	3623	1/1	0.94	0.37	64,64,64,64	0
56	MG	2A	3415	1/1	0.94	0.21	54,54,54,54	0
56	MG	2a	1667	1/1	0.94	0.10	56,56,56,56	0
56	MG	2A	3848	1/1	0.94	0.17	29,29,29,29	0
56	MG	1A	3114	1/1	0.94	0.35	39,39,39,39	0
56	MG	1A	3832	1/1	0.94	0.10	60,60,60,60	0
56	MG	2a	1673	1/1	0.94	0.17	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3234	1/1	0.94	0.64	35,35,35,35	0
56	MG	2a	1675	1/1	0.94	0.11	61,61,61,61	0
56	MG	2A	3852	1/1	0.94	0.77	50,50,50,50	0
56	MG	2A	3855	1/1	0.94	0.82	49,49,49,49	0
56	MG	2a	1680	1/1	0.94	0.17	58,58,58,58	0
56	MG	2a	1681	1/1	0.94	0.12	62,62,62,62	0
56	MG	1A	3725	1/1	0.94	0.13	53,53,53,53	0
56	MG	1A	3728	1/1	0.94	0.25	45,45,45,45	0
56	MG	1A	3836	1/1	0.94	0.12	62,62,62,62	0
56	MG	1A	3470	1/1	0.94	0.20	54,54,54,54	0
56	MG	2A	3634	1/1	0.94	0.14	41,41,41,41	0
56	MG	2A	3097	1/1	0.94	0.13	42,42,42,42	0
56	MG	1A	4071	1/1	0.94	0.11	55,55,55,55	0
56	MG	1A	3273	1/1	0.94	0.61	42,42,42,42	0
56	MG	2A	3103	1/1	0.94	0.13	27,27,27,27	0
56	MG	2A	3642	1/1	0.94	0.17	32,32,32,32	0
56	MG	1A	3732	1/1	0.94	0.12	23,23,23,23	0
56	MG	1A	3023	1/1	0.94	0.07	18,18,18,18	0
56	MG	1a	1762	1/1	0.94	0.09	62,62,62,62	0
56	MG	2A	3270	1/1	0.94	0.21	57,57,57,57	0
56	MG	2A	3434	1/1	0.94	0.22	41,41,41,41	0
56	MG	2a	1705	1/1	0.94	0.14	78,78,78,78	0
56	MG	1B	215	1/1	0.94	0.06	52,52,52,52	0
56	MG	2A	3106	1/1	0.94	0.19	49,49,49,49	0
56	MG	1a	1768	1/1	0.94	0.11	54,54,54,54	0
56	MG	2a	1710	1/1	0.94	0.13	62,62,62,62	0
56	MG	1B	219	1/1	0.94	0.14	31,31,31,31	0
56	MG	1A	3325	1/1	0.94	0.13	45,45,45,45	0
56	MG	1a	1771	1/1	0.94	0.08	59,59,59,59	0
56	MG	1A	3846	1/1	0.94	0.14	35,35,35,35	0
56	MG	2A	3439	1/1	0.94	0.10	65,65,65,65	0
56	MG	1A	3326	1/1	0.94	0.11	52,52,52,52	0
56	MG	1A	3081	1/1	0.94	0.46	39,39,39,39	0
56	MG	2A	3112	1/1	0.94	0.20	56,56,56,56	0
56	MG	1A	3740	1/1	0.94	0.15	44,44,44,44	0
56	MG	1B	228	1/1	0.94	0.11	39,39,39,39	0
56	MG	1A	3067	1/1	0.94	0.13	29,29,29,29	0
56	MG	1A	3744	1/1	0.94	0.09	25,25,25,25	0
56	MG	1A	3745	1/1	0.94	0.13	57,57,57,57	0
56	MG	2a	1724	1/1	0.94	0.24	57,57,57,57	0
56	MG	1A	3626	1/1	0.94	0.14	19,19,19,19	0
56	MG	1a	1783	1/1	0.94	0.08	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3371	1/1	0.94	0.14	46,46,46,46	0
56	MG	1A	3750	1/1	0.94	0.17	38,38,38,38	0
56	MG	1a	1788	1/1	0.94	0.15	57,57,57,57	0
56	MG	1A	3970	1/1	0.94	0.20	24,24,24,24	0
56	MG	1D	301	1/1	0.94	0.43	28,28,28,28	0
56	MG	1A	3628	1/1	0.94	0.12	25,25,25,25	0
56	MG	1D	305	1/1	0.94	0.55	34,34,34,34	0
56	MG	2A	3676	1/1	0.94	0.11	53,53,53,53	0
56	MG	1D	308	1/1	0.94	0.65	31,31,31,31	0
56	MG	1a	1796	1/1	0.94	0.10	42,42,42,42	0
56	MG	2A	3454	1/1	0.94	0.08	65,65,65,65	0
56	MG	1A	4105	1/1	0.94	0.42	30,30,30,30	0
56	MG	1a	1801	1/1	0.94	0.09	53,53,53,53	0
56	MG	2A	3680	1/1	0.94	0.14	53,53,53,53	0
56	MG	1E	301	1/1	0.94	0.14	35,35,35,35	0
56	MG	2A	3681	1/1	0.94	0.07	55,55,55,55	0
56	MG	2A	3126	1/1	0.94	0.07	47,47,47,47	0
56	MG	2a	1745	1/1	0.94	0.12	54,54,54,54	0
56	MG	2A	3683	1/1	0.94	0.11	78,78,78,78	0
56	MG	1A	3149	1/1	0.94	0.53	43,43,43,43	0
56	MG	1A	3182	1/1	0.94	0.08	68,68,68,68	0
56	MG	1a	1811	1/1	0.94	0.09	60,60,60,60	0
56	MG	1A	3209	1/1	0.94	0.22	42,42,42,42	0
56	MG	2A	3687	1/1	0.94	0.17	28,28,28,28	0
56	MG	1F	307	1/1	0.94	0.50	34,34,34,34	0
56	MG	1A	3334	1/1	0.94	0.08	43,43,43,43	0
56	MG	1A	3377	1/1	0.94	0.10	44,44,44,44	0
56	MG	1A	3551	1/1	0.94	0.24	46,46,46,46	0
56	MG	2A	3134	1/1	0.94	0.12	32,32,32,32	0
56	MG	1A	4119	1/1	0.94	0.50	35,35,35,35	0
56	MG	1A	3485	1/1	0.94	0.39	38,38,38,38	0
56	MG	1A	4121	1/1	0.94	0.51	27,27,27,27	0
56	MG	1A	3429	1/1	0.94	0.16	53,53,53,53	0
56	MG	1N	201	1/1	0.94	0.23	48,48,48,48	0
56	MG	2A	3474	1/1	0.94	0.15	34,34,34,34	0
56	MG	1A	3763	1/1	0.94	0.15	16,16,16,16	0
56	MG	1A	3098	1/1	0.94	0.14	34,34,34,34	0
56	MG	1A	3645	1/1	0.94	0.16	37,37,37,37	0
56	MG	1A	3068	1/1	0.94	0.23	64,64,64,64	0
56	MG	1A	3984	1/1	0.94	0.12	40,40,40,40	0
56	MG	1O	204	1/1	0.94	0.35	51,51,51,51	0
56	MG	1A	3985	1/1	0.94	0.19	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	3148	1/1	0.94	0.19	50,50,50,50	0
56	MG	1a	1841	1/1	0.94	0.17	62,62,62,62	0
56	MG	2a	1781	1/1	0.94	0.19	55,55,55,55	0
56	MG	1A	4137	1/1	0.94	0.31	28,28,28,28	0
56	MG	2a	1784	1/1	0.94	0.54	74,74,74,74	0
56	MG	1A	3649	1/1	0.94	0.13	33,33,33,33	0
56	MG	1A	3288	1/1	0.94	0.48	55,55,55,55	0
56	MG	2A	3710	1/1	0.94	0.18	61,61,61,61	0
56	MG	1A	3651	1/1	0.94	0.12	55,55,55,55	0
56	MG	2A	3489	1/1	0.94	0.24	41,41,41,41	0
56	MG	1S	202	1/1	0.94	0.24	45,45,45,45	0
56	MG	1A	3214	1/1	0.94	0.65	48,48,48,48	0
56	MG	2A	3159	1/1	0.94	0.15	71,71,71,71	0
56	MG	1A	3876	1/1	0.94	0.21	21,21,21,21	0
56	MG	1A	3877	1/1	0.94	0.18	45,45,45,45	0
56	MG	2A	3720	1/1	0.94	0.23	69,69,69,69	0
56	MG	1U	204	1/1	0.94	0.81	34,34,34,34	0
56	MG	1A	3655	1/1	0.94	0.14	14,14,14,14	0
56	MG	2A	3497	1/1	0.94	0.10	47,47,47,47	0
56	MG	1V	202	1/1	0.94	0.19	68,68,68,68	0
56	MG	2A	3725	1/1	0.94	0.10	49,49,49,49	0
56	MG	2A	3321	1/1	0.94	0.15	48,48,48,48	0
56	MG	1w	104	1/1	0.94	0.28	55,55,55,55	0
56	MG	1A	3882	1/1	0.94	0.14	20,20,20,20	0
56	MG	1A	3997	1/1	0.94	0.27	37,37,37,37	0
56	MG	1A	3085	1/1	0.94	0.38	36,36,36,36	0
56	MG	1Z	301	1/1	0.94	0.26	48,48,48,48	0
56	MG	1A	3493	1/1	0.94	0.55	42,42,42,42	0
56	MG	1A	4001	1/1	0.94	0.09	30,30,30,30	0
56	MG	1A	3776	1/1	0.94	0.09	54,54,54,54	0
56	MG	1A	3659	1/1	0.94	0.18	17,17,17,17	0
56	MG	1x	110	1/1	0.94	0.16	49,49,49,49	0
56	MG	1A	3778	1/1	0.94	0.15	16,16,16,16	0
56	MG	2A	3175	1/1	0.94	0.24	59,59,59,59	0
56	MG	1A	3155	1/1	0.94	0.94	40,40,40,40	0
56	MG	12	102	1/1	0.94	0.47	39,39,39,39	0
56	MG	1A	3892	1/1	0.94	0.17	43,43,43,43	0
56	MG	13	102	1/1	0.94	0.47	41,41,41,41	0
56	MG	2A	3178	1/1	0.94	0.14	44,44,44,44	0
56	MG	1A	3156	1/1	0.94	0.19	30,30,30,30	0
56	MG	2A	3743	1/1	0.94	0.18	35,35,35,35	0
56	MG	1A	3087	1/1	0.94	1.00	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3783	1/1	0.94	0.19	18,18,18,18	0
56	MG	16	101	1/1	0.94	0.35	52,52,52,52	0
56	MG	2A	3184	1/1	0.94	0.23	72,72,72,72	0
56	MG	1A	3569	1/1	0.94	0.13	59,59,59,59	0
56	MG	2A	3186	1/1	0.94	0.17	56,56,56,56	0
56	MG	2A	3187	1/1	0.94	0.08	45,45,45,45	0
56	MG	1A	3497	1/1	0.94	0.25	53,53,53,53	0
56	MG	1A	3191	1/1	0.94	0.61	34,34,34,34	0
56	MG	2B	216	1/1	0.94	0.20	69,69,69,69	0
56	MG	2A	3349	1/1	0.94	0.13	69,69,69,69	0
56	MG	1A	3499	1/1	0.94	0.49	42,42,42,42	0
56	MG	2q	202	1/1	0.94	0.10	67,67,67,67	0
56	MG	1A	3103	1/1	0.94	0.17	60,60,60,60	0
56	MG	2B	221	1/1	0.94	0.06	82,82,82,82	0
56	MG	2t	201	1/1	0.94	0.10	56,56,56,56	0
56	MG	1A	3221	1/1	0.94	0.53	39,39,39,39	0
56	MG	2A	3527	1/1	0.94	0.36	66,66,66,66	0
56	MG	1a	1612	1/1	0.94	0.14	59,59,59,59	0
56	MG	2A	3528	1/1	0.94	0.12	70,70,70,70	0
56	MG	1A	3576	1/1	0.94	0.16	40,40,40,40	0
56	MG	1A	4019	1/1	0.94	0.08	44,44,44,44	0
56	MG	1A	3673	1/1	0.94	0.09	51,51,51,51	0
56	MG	2A	3356	1/1	0.94	0.20	64,64,64,64	0
56	MG	1A	3006	1/1	0.94	0.14	51,51,51,51	0
56	MG	2A	3537	1/1	0.94	0.15	69,69,69,69	0
56	MG	1A	4024	1/1	0.94	0.32	66,66,66,66	0
56	MG	2A	3541	1/1	0.94	0.11	54,54,54,54	0
56	MG	1A	3507	1/1	0.94	0.41	32,32,32,32	0
57	DI0	2A	3846	58/58	0.94	0.43	33,44,84,93	0
56	MG	1A	3797	1/1	0.94	0.19	59,59,59,59	0
56	MG	2A	3200	1/1	0.94	0.54	47,47,47,47	0
56	MG	1A	3798	1/1	0.94	0.51	52,52,52,52	0
56	MG	2A	3549	1/1	0.94	0.13	58,58,58,58	0
56	MG	1A	3196	1/1	0.94	0.13	36,36,36,36	0
56	MG	2A	3157	1/1	0.95	0.19	28,28,28,28	0
56	MG	2A	3022	1/1	0.95	0.12	47,47,47,47	0
56	MG	2a	1638	1/1	0.95	0.22	62,62,62,62	0
56	MG	1A	3187	1/1	0.95	0.57	42,42,42,42	0
56	MG	2A	3581	1/1	0.95	0.16	43,43,43,43	0
56	MG	1P	203	1/1	0.95	0.40	29,29,29,29	0
56	MG	1Q	201	1/1	0.95	0.18	37,37,37,37	0
56	MG	1A	3011	1/1	0.95	0.13	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3161	1/1	0.95	0.15	42,42,42,42	0
56	MG	1A	3955	1/1	0.95	0.26	33,33,33,33	0
56	MG	2a	1646	1/1	0.95	0.29	57,57,57,57	0
56	MG	1A	3690	1/1	0.95	0.14	34,34,34,34	0
56	MG	1A	3619	1/1	0.95	0.15	31,31,31,31	0
56	MG	2A	3432	1/1	0.95	0.14	33,33,33,33	0
56	MG	2A	3028	1/1	0.95	0.10	52,52,52,52	0
56	MG	1A	3556	1/1	0.95	0.81	37,37,37,37	0
56	MG	2A	3297	1/1	0.95	0.51	38,38,38,38	0
56	MG	1A	3108	1/1	0.95	0.82	35,35,35,35	0
56	MG	1A	3697	1/1	0.95	0.14	18,18,18,18	0
56	MG	1A	3698	1/1	0.95	0.27	28,28,28,28	0
56	MG	1A	4057	1/1	0.95	0.36	51,51,51,51	0
56	MG	1A	3500	1/1	0.95	0.07	58,58,58,58	0
56	MG	1A	3076	1/1	0.95	0.12	33,33,33,33	0
56	MG	1U	207	1/1	0.95	0.76	38,38,38,38	0
56	MG	1V	201	1/1	0.95	0.15	38,38,38,38	0
56	MG	2A	3599	1/1	0.95	0.11	66,66,66,66	0
56	MG	1W	202	1/1	0.95	0.12	35,35,35,35	0
56	MG	1W	204	1/1	0.95	0.74	39,39,39,39	0
56	MG	1W	205	1/1	0.95	0.47	39,39,39,39	0
56	MG	1A	3702	1/1	0.95	0.21	49,49,49,49	0
56	MG	1a	1791	1/1	0.95	0.19	75,75,75,75	0
56	MG	1A	3163	1/1	0.95	0.28	44,44,44,44	0
56	MG	2a	1669	1/1	0.95	0.12	63,63,63,63	0
56	MG	2A	3042	1/1	0.95	0.21	56,56,56,56	0
56	MG	1X	105	1/1	0.95	0.51	52,52,52,52	0
56	MG	2A	3043	1/1	0.95	0.27	63,63,63,63	0
56	MG	2A	3778	1/1	0.95	0.16	49,49,49,49	0
56	MG	1A	3458	1/1	0.95	0.18	39,39,39,39	0
56	MG	1a	1798	1/1	0.95	0.07	66,66,66,66	0
56	MG	1A	3165	1/1	0.95	0.49	35,35,35,35	0
56	MG	2A	3608	1/1	0.95	0.14	47,47,47,47	0
56	MG	10	101	1/1	0.95	0.08	38,38,38,38	0
56	MG	1a	1803	1/1	0.95	0.14	70,70,70,70	0
56	MG	10	102	1/1	0.95	0.10	56,56,56,56	0
56	MG	2A	3450	1/1	0.95	0.10	65,65,65,65	0
56	MG	1A	3460	1/1	0.95	0.84	43,43,43,43	0
56	MG	1A	3881	1/1	0.95	0.10	20,20,20,20	0
56	MG	1A	3566	1/1	0.95	0.22	40,40,40,40	0
56	MG	11	101	1/1	0.95	0.13	27,27,27,27	0
56	MG	11	104	1/1	0.95	0.13	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3633	1/1	0.95	0.06	43,43,43,43	0
56	MG	2A	3616	1/1	0.95	0.08	47,47,47,47	0
56	MG	2A	3619	1/1	0.95	0.11	35,35,35,35	0
56	MG	2a	1698	1/1	0.95	0.15	62,62,62,62	0
56	MG	2A	3455	1/1	0.95	0.06	79,79,79,79	0
56	MG	2a	1700	1/1	0.95	0.21	62,62,62,62	0
56	MG	1A	3370	1/1	0.95	0.15	46,46,46,46	0
56	MG	15	101	1/1	0.95	0.07	41,41,41,41	0
56	MG	1A	3712	1/1	0.95	0.16	46,46,46,46	0
56	MG	2a	1704	1/1	0.95	0.15	66,66,66,66	0
56	MG	1A	3886	1/1	0.95	0.09	49,49,49,49	0
56	MG	1A	3033	1/1	0.95	0.56	29,29,29,29	0
56	MG	1A	4073	1/1	0.95	0.16	34,34,34,34	0
56	MG	1A	4074	1/1	0.95	0.10	49,49,49,49	0
56	MG	2a	1709	1/1	0.95	0.10	71,71,71,71	0
56	MG	2A	3060	1/1	0.95	0.17	38,38,38,38	0
56	MG	2A	3629	1/1	0.95	0.21	49,49,49,49	0
56	MG	1A	4076	1/1	0.95	0.11	44,44,44,44	0
56	MG	1A	4078	1/1	0.95	0.19	45,45,45,45	0
56	MG	2A	3466	1/1	0.95	0.22	59,59,59,59	0
56	MG	1A	3806	1/1	0.95	0.28	25,25,25,25	0
56	MG	1A	3195	1/1	0.95	0.08	39,39,39,39	0
56	MG	2A	3066	1/1	0.95	0.27	51,51,51,51	0
56	MG	1a	1837	1/1	0.95	0.09	79,79,79,79	0
56	MG	2A	3637	1/1	0.95	0.10	57,57,57,57	0
56	MG	1A	3719	1/1	0.95	0.13	53,53,53,53	0
56	MG	1A	3005	1/1	0.95	0.34	47,47,47,47	0
56	MG	1a	1610	1/1	0.95	0.16	46,46,46,46	0
56	MG	1A	4085	1/1	0.95	0.10	50,50,50,50	0
56	MG	1a	1844	1/1	0.95	0.14	46,46,46,46	0
56	MG	2A	3333	1/1	0.95	0.29	59,59,59,59	0
56	MG	1a	1614	1/1	0.95	0.26	43,43,43,43	0
56	MG	1A	3895	1/1	0.95	0.12	42,42,42,42	0
56	MG	2A	3338	1/1	0.95	0.16	47,47,47,47	0
56	MG	1A	3727	1/1	0.95	0.15	36,36,36,36	0
56	MG	1A	3811	1/1	0.95	0.14	39,39,39,39	0
56	MG	1A	3040	1/1	0.95	0.28	57,57,57,57	0
56	MG	2A	3650	1/1	0.95	0.20	54,54,54,54	0
56	MG	1a	1622	1/1	0.95	0.14	59,59,59,59	0
56	MG	1A	3118	1/1	0.95	0.63	28,28,28,28	0
56	MG	1A	3901	1/1	0.95	0.13	19,19,19,19	0
56	MG	2A	3654	1/1	0.95	0.18	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	3079	1/1	0.95	0.07	45,45,45,45	0
56	MG	2A	3657	1/1	0.95	0.10	45,45,45,45	0
56	MG	2A	3080	1/1	0.95	0.30	39,39,39,39	0
56	MG	2A	3660	1/1	0.95	0.19	37,37,37,37	0
56	MG	2A	3661	1/1	0.95	0.21	44,44,44,44	0
56	MG	2A	3216	1/1	0.95	0.15	61,61,61,61	0
56	MG	1A	4096	1/1	0.95	0.12	56,56,56,56	0
56	MG	2A	3664	1/1	0.95	0.11	37,37,37,37	0
56	MG	1A	3259	1/1	0.95	0.13	60,60,60,60	0
56	MG	1x	103	1/1	0.95	0.19	66,66,66,66	0
56	MG	2A	3666	1/1	0.95	0.15	37,37,37,37	0
56	MG	2a	1750	1/1	0.95	0.16	61,61,61,61	0
56	MG	1A	3646	1/1	0.95	0.12	44,44,44,44	0
56	MG	1A	3991	1/1	0.95	0.06	68,68,68,68	0
56	MG	1A	3816	1/1	0.95	0.09	52,52,52,52	0
56	MG	1a	1641	1/1	0.95	0.58	52,52,52,52	0
56	MG	1A	3647	1/1	0.95	0.13	28,28,28,28	0
56	MG	1A	3818	1/1	0.95	0.20	43,43,43,43	0
56	MG	1A	3008	1/1	0.95	0.10	23,23,23,23	0
56	MG	1A	3380	1/1	0.95	0.55	38,38,38,38	0
56	MG	2A	3847	1/1	0.95	0.56	48,48,48,48	0
56	MG	1A	3301	1/1	0.95	0.13	40,40,40,40	0
56	MG	1a	1650	1/1	0.95	0.10	57,57,57,57	0
56	MG	2A	3098	1/1	0.95	0.21	44,44,44,44	0
56	MG	2A	3677	1/1	0.95	0.14	57,57,57,57	0
56	MG	1A	3053	1/1	0.95	0.37	51,51,51,51	0
56	MG	1A	3999	1/1	0.95	0.09	30,30,30,30	0
56	MG	2A	3853	1/1	0.95	0.20	53,53,53,53	0
56	MG	1A	4114	1/1	0.95	0.56	42,42,42,42	0
56	MG	1A	3652	1/1	0.95	0.15	37,37,37,37	0
56	MG	2a	1774	1/1	0.95	0.11	63,63,63,63	0
56	MG	2A	3234	1/1	0.95	0.33	60,60,60,60	0
56	MG	2a	1776	1/1	0.95	0.16	49,49,49,49	0
56	MG	1A	3176	1/1	0.95	0.15	26,26,26,26	0
56	MG	1a	1664	1/1	0.95	0.34	64,64,64,64	0
56	MG	1A	3915	1/1	0.95	0.17	52,52,52,52	0
56	MG	1A	3263	1/1	0.95	0.25	59,59,59,59	0
56	MG	1A	3474	1/1	0.95	0.32	41,41,41,41	0
56	MG	1B	202	1/1	0.95	0.19	59,59,59,59	0
56	MG	2A	3109	1/1	0.95	0.29	52,52,52,52	0
56	MG	1A	3346	1/1	0.95	0.23	50,50,50,50	0
56	MG	1A	3528	1/1	0.95	0.20	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	2D	302	1/1	0.95	0.70	47,47,47,47	0
56	MG	1B	206	1/1	0.95	0.08	44,44,44,44	0
56	MG	2A	3243	1/1	0.95	0.13	50,50,50,50	0
56	MG	1A	4007	1/1	0.95	0.11	54,54,54,54	0
56	MG	2A	3692	1/1	0.95	0.16	40,40,40,40	0
56	MG	1a	1679	1/1	0.95	0.35	47,47,47,47	0
56	MG	2A	3113	1/1	0.95	0.13	50,50,50,50	0
56	MG	1A	3042	1/1	0.95	0.37	28,28,28,28	0
56	MG	2a	1799	1/1	0.95	0.21	56,56,56,56	0
56	MG	2A	3115	1/1	0.95	0.40	40,40,40,40	0
56	MG	1A	3661	1/1	0.95	0.14	17,17,17,17	0
56	MG	1B	218	1/1	0.95	0.17	42,42,42,42	0
56	MG	1A	4010	1/1	0.95	0.12	63,63,63,63	0
56	MG	1A	3753	1/1	0.95	0.26	26,26,26,26	0
56	MG	1a	1690	1/1	0.95	0.19	40,40,40,40	0
56	MG	1a	1691	1/1	0.95	0.07	62,62,62,62	0
56	MG	2P	202	1/1	0.95	0.18	47,47,47,47	0
56	MG	1A	3924	1/1	0.95	0.09	57,57,57,57	0
56	MG	1A	3003	1/1	0.95	0.18	20,20,20,20	0
56	MG	1A	3180	1/1	0.95	0.14	47,47,47,47	0
56	MG	1A	3152	1/1	0.95	0.15	35,35,35,35	0
56	MG	1A	3838	1/1	0.95	0.11	46,46,46,46	0
56	MG	2A	3124	1/1	0.95	0.17	44,44,44,44	0
56	MG	2A	3533	1/1	0.95	0.11	59,59,59,59	0
56	MG	1A	3930	1/1	0.95	0.10	47,47,47,47	0
56	MG	1a	1701	1/1	0.95	0.22	46,46,46,46	0
56	MG	2a	1820	1/1	0.95	0.20	57,57,57,57	0
56	MG	1A	3235	1/1	0.95	0.47	26,26,26,26	0
56	MG	2U	203	1/1	0.95	1.05	58,58,58,58	0
56	MG	2A	3261	1/1	0.95	0.14	41,41,41,41	0
56	MG	1B	232	1/1	0.95	0.08	65,65,65,65	0
56	MG	2A	3538	1/1	0.95	0.14	29,29,29,29	0
56	MG	1a	1709	1/1	0.95	0.20	41,41,41,41	0
56	MG	1A	3593	1/1	0.95	0.36	34,34,34,34	0
56	MG	1A	3072	1/1	0.95	0.82	36,36,36,36	0
56	MG	1A	3313	1/1	0.95	0.12	47,47,47,47	0
56	MG	2A	3715	1/1	0.95	0.09	54,54,54,54	0
56	MG	2A	3716	1/1	0.95	0.16	41,41,41,41	0
56	MG	2A	3544	1/1	0.95	0.21	64,64,64,64	0
56	MG	1A	3237	1/1	0.95	0.34	40,40,40,40	0
56	MG	1A	3315	1/1	0.95	0.49	36,36,36,36	0
56	MG	2A	3722	1/1	0.95	0.16	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	3154	1/1	0.95	0.12	44,44,44,44	0
56	MG	2A	3399	1/1	0.95	0.15	43,43,43,43	0
56	MG	1a	1722	1/1	0.95	0.29	59,59,59,59	0
56	MG	1A	4027	1/1	0.95	0.30	58,58,58,58	0
56	MG	1a	1725	1/1	0.95	0.18	46,46,46,46	0
56	MG	1A	3318	1/1	0.95	0.28	32,32,32,32	0
56	MG	1A	3675	1/1	0.95	0.19	22,22,22,22	0
56	MG	1A	3056	1/1	0.95	0.16	34,34,34,34	0
56	MG	2A	3557	1/1	0.95	0.19	56,56,56,56	0
56	MG	1A	3942	1/1	0.95	0.18	43,43,43,43	0
56	MG	1A	3446	1/1	0.95	0.16	59,59,59,59	0
56	MG	1A	3447	1/1	0.95	0.28	36,36,36,36	0
56	MG	1a	1736	1/1	0.95	0.18	34,34,34,34	0
56	MG	1F	306	1/1	0.95	0.74	27,27,27,27	0
56	MG	2A	3563	1/1	0.95	0.10	45,45,45,45	0
56	MG	2A	3013	1/1	0.95	0.18	37,37,37,37	0
56	MG	2A	3736	1/1	0.95	0.11	59,59,59,59	0
56	MG	1A	3491	1/1	0.95	0.66	34,34,34,34	0
56	MG	1A	3609	1/1	0.95	0.18	45,45,45,45	0
56	MG	1A	3243	1/1	0.95	0.20	51,51,51,51	0
56	MG	2A	3147	1/1	0.95	0.36	48,48,48,48	0
56	MG	2A	3414	1/1	0.95	0.12	66,66,66,66	0
56	MG	2A	3017	1/1	0.95	0.30	53,53,53,53	0
56	MG	1A	3106	1/1	0.95	0.41	34,34,34,34	0
58	K	1A	4145	1/1	0.95	0.09	55,55,55,55	0
56	MG	2A	3150	1/1	0.95	0.09	40,40,40,40	0
56	MG	1A	3277	1/1	0.95	0.45	31,31,31,31	0
56	MG	1A	3245	1/1	0.95	0.08	43,43,43,43	0
56	MG	2A	3575	1/1	0.95	0.14	35,35,35,35	0
56	MG	1A	3213	1/1	0.95	0.15	40,40,40,40	0
56	MG	2A	3607	1/1	0.96	0.11	27,27,27,27	0
56	MG	1A	3127	1/1	0.96	0.31	35,35,35,35	0
56	MG	1A	3519	1/1	0.96	0.10	45,45,45,45	0
56	MG	2A	3055	1/1	0.96	0.21	44,44,44,44	0
56	MG	2a	1672	1/1	0.96	0.20	40,40,40,40	0
56	MG	1A	3520	1/1	0.96	0.34	47,47,47,47	0
56	MG	2A	3613	1/1	0.96	0.14	34,34,34,34	0
56	MG	1A	3311	1/1	0.96	0.07	41,41,41,41	0
56	MG	2A	3483	1/1	0.96	0.26	49,49,49,49	0
56	MG	1a	1840	1/1	0.96	0.07	54,54,54,54	0
56	MG	1a	1652	1/1	0.96	0.17	48,48,48,48	0
56	MG	2A	3153	1/1	0.96	0.23	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	1B	236	1/1	0.96	0.13	37,37,37,37	0
56	MG	1A	3111	1/1	0.96	0.15	38,38,38,38	0
56	MG	2A	3156	1/1	0.96	0.10	51,51,51,51	0
56	MG	1A	3279	1/1	0.96	0.95	34,34,34,34	0
56	MG	2a	1686	1/1	0.96	0.17	55,55,55,55	0
56	MG	2a	1687	1/1	0.96	0.25	70,70,70,70	0
56	MG	2A	3488	1/1	0.96	0.23	48,48,48,48	0
56	MG	2a	1690	1/1	0.96	0.23	53,53,53,53	0
56	MG	1A	4118	1/1	0.96	0.56	35,35,35,35	0
56	MG	1A	3620	1/1	0.96	0.11	44,44,44,44	0
56	MG	1a	1663	1/1	0.96	0.11	45,45,45,45	0
56	MG	2a	1694	1/1	0.96	0.17	51,51,51,51	0
56	MG	1A	3043	1/1	0.96	0.35	27,27,27,27	0
56	MG	1A	3571	1/1	0.96	0.09	35,35,35,35	0
56	MG	2A	3759	1/1	0.96	0.12	54,54,54,54	0
56	MG	2A	3760	1/1	0.96	0.51	52,52,52,52	0
56	MG	2A	3374	1/1	0.96	0.41	61,61,61,61	0
56	MG	2A	3065	1/1	0.96	0.19	54,54,54,54	0
56	MG	1E	304	1/1	0.96	0.55	51,51,51,51	0
56	MG	1A	4034	1/1	0.96	0.21	25,25,25,25	0
56	MG	1a	1672	1/1	0.96	0.24	49,49,49,49	0
56	MG	1A	3681	1/1	0.96	0.14	31,31,31,31	0
56	MG	1w	103	1/1	0.96	0.18	75,75,75,75	0
56	MG	1E	308	1/1	0.96	0.13	43,43,43,43	0
56	MG	1A	4036	1/1	0.96	0.10	35,35,35,35	0
56	MG	2A	3274	1/1	0.96	0.09	44,44,44,44	0
56	MG	1A	3824	1/1	0.96	0.12	24,24,24,24	0
56	MG	2A	3383	1/1	0.96	0.13	51,51,51,51	0
56	MG	1a	1681	1/1	0.96	0.21	42,42,42,42	0
56	MG	1a	1682	1/1	0.96	0.24	36,36,36,36	0
56	MG	2A	3636	1/1	0.96	0.19	62,62,62,62	0
56	MG	1x	106	1/1	0.96	0.10	66,66,66,66	0
56	MG	1A	3825	1/1	0.96	0.10	52,52,52,52	0
56	MG	1A	3624	1/1	0.96	0.08	38,38,38,38	0
56	MG	1A	4130	1/1	0.96	1.23	39,39,39,39	0
56	MG	1A	4131	1/1	0.96	0.83	42,42,42,42	0
56	MG	2A	3641	1/1	0.96	0.09	51,51,51,51	0
56	MG	1A	4133	1/1	0.96	1.18	28,28,28,28	0
56	MG	2A	3075	1/1	0.96	0.08	40,40,40,40	0
56	MG	1A	4134	1/1	0.96	0.56	29,29,29,29	0
56	MG	1I	201	1/1	0.96	0.14	60,60,60,60	0
56	MG	2A	3078	1/1	0.96	0.29	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	2A	3780	1/1	0.96	0.11	35,35,35,35	0
56	MG	1A	3253	1/1	0.96	0.15	36,36,36,36	0
56	MG	2B	204	1/1	0.96	0.16	75,75,75,75	0
56	MG	2B	205	1/1	0.96	0.17	69,69,69,69	0
56	MG	1N	204	1/1	0.96	0.39	46,46,46,46	0
56	MG	1N	205	1/1	0.96	0.86	44,44,44,44	0
56	MG	1N	206	1/1	0.96	0.19	34,34,34,34	0
56	MG	2A	3648	1/1	0.96	0.13	31,31,31,31	0
56	MG	2A	3783	1/1	0.96	0.12	48,48,48,48	0
56	MG	1a	1703	1/1	0.96	0.14	38,38,38,38	0
56	MG	1A	3070	1/1	0.96	0.16	19,19,19,19	0
56	MG	1A	3157	1/1	0.96	0.11	63,63,63,63	0
56	MG	2A	3082	1/1	0.96	0.13	59,59,59,59	0
56	MG	1O	205	1/1	0.96	0.10	58,58,58,58	0
56	MG	2A	3083	1/1	0.96	0.12	36,36,36,36	0
56	MG	1A	3764	1/1	0.96	0.07	36,36,36,36	0
56	MG	2A	3655	1/1	0.96	0.12	59,59,59,59	0
56	MG	2A	3398	1/1	0.96	0.07	56,56,56,56	0
56	MG	1A	3184	1/1	0.96	0.28	40,40,40,40	0
56	MG	2A	3658	1/1	0.96	0.09	51,51,51,51	0
56	MG	2A	3086	1/1	0.96	0.29	58,58,58,58	0
56	MG	2A	3401	1/1	0.96	0.30	46,46,46,46	0
56	MG	2A	3087	1/1	0.96	0.09	29,29,29,29	0
56	MG	2A	3797	1/1	0.96	0.17	32,32,32,32	0
56	MG	1A	3028	1/1	0.96	0.17	68,68,68,68	0
56	MG	1A	3532	1/1	0.96	0.28	40,40,40,40	0
56	MG	1A	3387	1/1	0.96	0.76	34,34,34,34	0
56	MG	2A	3092	1/1	0.96	0.10	35,35,35,35	0
56	MG	1U	201	1/1	0.96	0.55	37,37,37,37	0
56	MG	1A	3208	1/1	0.96	0.15	35,35,35,35	0
56	MG	2A	3408	1/1	0.96	0.30	62,62,62,62	0
56	MG	2a	1759	1/1	0.96	0.11	61,61,61,61	0
56	MG	2A	3298	1/1	0.96	0.56	50,50,50,50	0
56	MG	2A	3094	1/1	0.96	0.25	67,67,67,67	0
56	MG	1A	3159	1/1	0.96	0.61	33,33,33,33	0
56	MG	2A	3301	1/1	0.96	0.56	54,54,54,54	0
56	MG	2A	3536	1/1	0.96	0.13	42,42,42,42	0
56	MG	2A	3810	1/1	0.96	0.18	51,51,51,51	0
56	MG	2Q	202	1/1	0.96	0.19	41,41,41,41	0
56	MG	1W	201	1/1	0.96	0.22	44,44,44,44	0
56	MG	1A	3635	1/1	0.96	0.16	47,47,47,47	0
56	MG	1W	203	1/1	0.96	0.55	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	1771	1/1	0.96	0.12	54,54,54,54	0
56	MG	1A	4150	1/1	0.96	0.15	38,38,38,38	0
56	MG	1a	1744	1/1	0.96	0.11	36,36,36,36	0
56	MG	1A	3135	1/1	0.96	0.26	30,30,30,30	0
56	MG	2A	3099	1/1	0.96	0.10	46,46,46,46	0
56	MG	2A	3542	1/1	0.96	0.15	44,44,44,44	0
56	MG	2A	3306	1/1	0.96	0.15	70,70,70,70	0
56	MG	2A	3100	1/1	0.96	0.13	36,36,36,36	0
56	MG	1A	3841	1/1	0.96	0.14	47,47,47,47	0
56	MG	2A	3546	1/1	0.96	0.10	66,66,66,66	0
56	MG	1A	3116	1/1	0.96	0.64	34,34,34,34	0
56	MG	2A	3821	1/1	0.96	0.10	28,28,28,28	0
56	MG	1a	1756	1/1	0.96	0.10	66,66,66,66	0
56	MG	2X	102	1/1	0.96	0.32	57,57,57,57	0
56	MG	2Z	301	1/1	0.96	0.12	74,74,74,74	0
56	MG	2a	1791	1/1	0.96	0.08	71,71,71,71	0
56	MG	20	101	1/1	0.96	0.20	53,53,53,53	0
56	MG	2A	3204	1/1	0.96	0.19	53,53,53,53	0
56	MG	1a	1758	1/1	0.96	0.16	49,49,49,49	0
56	MG	1A	3035	1/1	0.96	0.34	41,41,41,41	0
56	MG	25	103	1/1	0.96	0.52	51,51,51,51	0
56	MG	1A	3640	1/1	0.96	0.21	25,25,25,25	0
56	MG	2A	3826	1/1	0.96	0.11	32,32,32,32	0
56	MG	1A	3061	1/1	0.96	0.25	35,35,35,35	0
56	MG	2A	3314	1/1	0.96	0.12	51,51,51,51	0
56	MG	1A	3327	1/1	0.96	0.11	55,55,55,55	0
56	MG	1A	3143	1/1	0.96	0.45	38,38,38,38	0
56	MG	11	102	1/1	0.96	0.20	42,42,42,42	0
56	MG	1A	3241	1/1	0.96	0.36	47,47,47,47	0
56	MG	2a	1805	1/1	0.96	0.21	63,63,63,63	0
56	MG	1A	3590	1/1	0.96	0.54	34,34,34,34	0
56	MG	1A	3925	1/1	0.96	0.11	23,23,23,23	0
56	MG	1A	3501	1/1	0.96	0.61	39,39,39,39	0
56	MG	1A	3242	1/1	0.96	0.19	47,47,47,47	0
56	MG	2a	1810	1/1	0.96	0.10	76,76,76,76	0
56	MG	1A	3503	1/1	0.96	0.56	56,56,56,56	0
56	MG	1A	3546	1/1	0.96	0.54	38,38,38,38	0
56	MG	2A	3438	1/1	0.96	0.19	68,68,68,68	0
56	MG	1A	3713	1/1	0.96	0.12	20,20,20,20	0
56	MG	2A	3221	1/1	0.96	0.27	36,36,36,36	0
56	MG	2a	1816	1/1	0.96	0.12	67,67,67,67	0
56	MG	1A	3331	1/1	0.96	0.19	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	3716	1/1	0.96	0.12	51,51,51,51	0
56	MG	2A	3704	1/1	0.96	0.22	70,70,70,70	0
56	MG	1A	3791	1/1	0.96	0.08	40,40,40,40	0
56	MG	1A	3435	1/1	0.96	0.23	50,50,50,50	0
56	MG	2a	1621	1/1	0.96	0.42	64,64,64,64	0
56	MG	1A	3718	1/1	0.96	0.11	39,39,39,39	0
56	MG	1a	1784	1/1	0.96	0.05	58,58,58,58	0
56	MG	1A	3597	1/1	0.96	0.10	52,52,52,52	0
56	MG	1A	3145	1/1	0.96	0.48	24,24,24,24	0
56	MG	1A	3657	1/1	0.96	0.14	44,44,44,44	0
56	MG	2a	1828	1/1	0.96	0.17	41,41,41,41	0
56	MG	2A	3578	1/1	0.96	0.07	55,55,55,55	0
56	MG	1A	3268	1/1	0.96	0.48	43,43,43,43	0
56	MG	1A	3601	1/1	0.96	0.20	38,38,38,38	0
56	MG	1A	3439	1/1	0.96	0.43	42,42,42,42	0
56	MG	1A	3802	1/1	0.96	0.20	53,53,53,53	0
56	MG	1a	1611	1/1	0.96	0.15	23,23,23,23	0
56	MG	2a	1634	1/1	0.96	0.15	47,47,47,47	0
56	MG	2A	3859	1/1	0.96	0.20	47,47,47,47	0
56	MG	1A	3603	1/1	0.96	0.19	31,31,31,31	0
56	MG	2A	3861	1/1	0.96	0.18	45,45,45,45	0
56	MG	1A	3733	1/1	0.96	0.54	31,31,31,31	0
56	MG	1A	3089	1/1	0.96	0.37	47,47,47,47	0
56	MG	1A	4094	1/1	0.96	0.16	42,42,42,42	0
56	MG	2A	3721	1/1	0.96	0.11	69,69,69,69	0
56	MG	1A	3036	1/1	0.96	0.26	27,27,27,27	0
56	MG	1a	1620	1/1	0.96	0.13	44,44,44,44	0
56	MG	1A	3606	1/1	0.96	0.15	28,28,28,28	0
56	MG	2A	3135	1/1	0.96	0.10	43,43,43,43	0
56	MG	1a	1623	1/1	0.96	0.10	54,54,54,54	0
56	MG	1A	3305	1/1	0.96	0.14	40,40,40,40	0
56	MG	1a	1809	1/1	0.96	0.09	45,45,45,45	0
56	MG	2x	101	1/1	0.96	0.12	57,57,57,57	0
56	MG	1A	3038	1/1	0.96	1.03	36,36,36,36	0
56	MG	1A	3079	1/1	0.96	0.14	27,27,27,27	0
56	MG	1B	211	1/1	0.96	0.26	57,57,57,57	0
56	MG	1A	3065	1/1	0.96	0.18	35,35,35,35	0
56	MG	1B	213	1/1	0.96	0.17	49,49,49,49	0
56	MG	2A	3729	1/1	0.96	0.15	26,26,26,26	0
56	MG	1A	3048	1/1	0.96	0.18	23,23,23,23	0
56	MG	1a	1820	1/1	0.96	0.08	61,61,61,61	0
56	MG	1A	4103	1/1	0.96	0.77	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	2A	3142	1/1	0.96	0.18	32,32,32,32	0
57	DI0	1A	4098	58/58	0.96	0.33	17,33,66,81	0
56	MG	1A	4104	1/1	0.96	0.65	31,31,31,31	0
56	MG	2A	3472	1/1	0.96	0.14	56,56,56,56	0
56	MG	1A	3747	1/1	0.96	0.16	47,47,47,47	0
59	ZN	1Y	204	1/1	0.96	0.07	84,84,84,84	0
56	MG	1A	4023	1/1	0.96	0.11	39,39,39,39	0
56	MG	2A	3475	1/1	0.96	0.12	51,51,51,51	0
56	MG	1A	4107	1/1	0.96	0.20	22,22,22,22	0
56	MG	1A	4108	1/1	0.96	0.93	30,30,30,30	0
56	MG	1B	216	1/1	0.97	0.19	38,38,38,38	0
56	MG	17	103	1/1	0.97	0.13	41,41,41,41	0
56	MG	1A	3049	1/1	0.97	0.11	38,38,38,38	0
56	MG	1A	3795	1/1	0.97	0.13	27,27,27,27	0
56	MG	2B	220	1/1	0.97	0.20	63,63,63,63	0
56	MG	1A	3239	1/1	0.97	0.80	29,29,29,29	0
56	MG	1A	3479	1/1	0.97	0.15	45,45,45,45	0
56	MG	1a	1752	1/1	0.97	0.14	43,43,43,43	0
56	MG	1a	1604	1/1	0.97	0.19	53,53,53,53	0
56	MG	1A	3858	1/1	0.97	0.16	30,30,30,30	0
56	MG	2E	302	1/1	0.97	0.24	39,39,39,39	0
56	MG	2A	3011	1/1	0.97	0.21	47,47,47,47	0
56	MG	1A	3009	1/1	0.97	0.08	17,17,17,17	0
56	MG	1A	3124	1/1	0.97	0.13	35,35,35,35	0
56	MG	1A	3013	1/1	0.97	0.74	26,26,26,26	0
56	MG	2E	307	1/1	0.97	0.18	49,49,49,49	0
56	MG	1A	3379	1/1	0.97	0.30	20,20,20,20	0
56	MG	1A	4075	1/1	0.97	0.17	36,36,36,36	0
56	MG	2A	3209	1/1	0.97	0.15	49,49,49,49	0
56	MG	1A	3741	1/1	0.97	0.06	38,38,38,38	0
56	MG	2A	3211	1/1	0.97	0.20	32,32,32,32	0
56	MG	2a	1725	1/1	0.97	0.13	48,48,48,48	0
56	MG	1a	1765	1/1	0.97	0.06	60,60,60,60	0
56	MG	1A	3598	1/1	0.97	0.15	39,39,39,39	0
56	MG	2O	202	1/1	0.97	0.12	55,55,55,55	0
56	MG	2A	3652	1/1	0.97	0.14	26,26,26,26	0
56	MG	2A	3532	1/1	0.97	0.14	56,56,56,56	0
56	MG	1A	3743	1/1	0.97	0.13	23,23,23,23	0
56	MG	1A	4080	1/1	0.97	0.08	58,58,58,58	0
56	MG	2A	3773	1/1	0.97	0.20	59,59,59,59	0
56	MG	1A	3866	1/1	0.97	0.49	28,28,28,28	0
56	MG	1A	4082	1/1	0.97	0.10	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	3160	1/1	0.97	0.65	32,32,32,32	0
56	MG	1A	3642	1/1	0.97	0.12	33,33,33,33	0
56	MG	1A	3938	1/1	0.97	0.10	49,49,49,49	0
56	MG	2A	3540	1/1	0.97	0.12	23,23,23,23	0
56	MG	1A	3686	1/1	0.97	0.13	17,17,17,17	0
56	MG	2A	3428	1/1	0.97	0.26	58,58,58,58	0
56	MG	2A	3429	1/1	0.97	0.11	52,52,52,52	0
56	MG	1a	1630	1/1	0.97	0.13	36,36,36,36	0
56	MG	1A	4087	1/1	0.97	0.07	48,48,48,48	0
56	MG	1A	3066	1/1	0.97	0.07	53,53,53,53	0
56	MG	2A	3667	1/1	0.97	0.20	45,45,45,45	0
56	MG	1A	4089	1/1	0.97	0.23	30,30,30,30	0
56	MG	1A	3147	1/1	0.97	0.31	45,45,45,45	0
56	MG	1A	3294	1/1	0.97	0.15	28,28,28,28	0
56	MG	2a	1751	1/1	0.97	0.19	58,58,58,58	0
56	MG	1A	3078	1/1	0.97	0.55	31,31,31,31	0
56	MG	2A	3034	1/1	0.97	0.28	34,34,34,34	0
56	MG	20	102	1/1	0.97	0.06	65,65,65,65	0
56	MG	1F	303	1/1	0.97	0.86	36,36,36,36	0
56	MG	1F	304	1/1	0.97	0.56	52,52,52,52	0
56	MG	2A	3035	1/1	0.97	0.30	39,39,39,39	0
56	MG	25	102	1/1	0.97	0.70	43,43,43,43	0
56	MG	2A	3553	1/1	0.97	0.12	42,42,42,42	0
56	MG	2A	3229	1/1	0.97	0.10	56,56,56,56	0
56	MG	2A	3794	1/1	0.97	0.13	79,79,79,79	0
56	MG	1A	4093	1/1	0.97	0.17	42,42,42,42	0
56	MG	1A	3164	1/1	0.97	0.54	32,32,32,32	0
56	MG	2a	1764	1/1	0.97	0.05	65,65,65,65	0
56	MG	1A	3875	1/1	0.97	0.12	28,28,28,28	0
56	MG	1A	3297	1/1	0.97	0.29	32,32,32,32	0
56	MG	2A	3444	1/1	0.97	0.39	57,57,57,57	0
56	MG	2A	3132	1/1	0.97	0.24	54,54,54,54	0
56	MG	1A	3052	1/1	0.97	0.17	36,36,36,36	0
56	MG	1a	1655	1/1	0.97	0.11	53,53,53,53	0
56	MG	1A	3694	1/1	0.97	0.14	15,15,15,15	0
56	MG	2a	1772	1/1	0.97	0.07	59,59,59,59	0
56	MG	1A	3695	1/1	0.97	0.12	16,16,16,16	0
56	MG	2a	1610	1/1	0.97	0.08	61,61,61,61	0
56	MG	1A	3696	1/1	0.97	0.09	37,37,37,37	0
56	MG	1A	3758	1/1	0.97	0.14	34,34,34,34	0
56	MG	2A	3806	1/1	0.97	0.09	74,74,74,74	0
56	MG	2A	3240	1/1	0.97	0.14	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	3046	1/1	0.97	0.18	49,49,49,49	0
56	MG	1A	3299	1/1	0.97	0.17	32,32,32,32	0
56	MG	2A	3048	1/1	0.97	0.17	52,52,52,52	0
56	MG	1a	1815	1/1	0.97	0.13	58,58,58,58	0
56	MG	1A	3953	1/1	0.97	0.09	34,34,34,34	0
56	MG	1A	3226	1/1	0.97	0.56	39,39,39,39	0
56	MG	2a	1786	1/1	0.97	0.15	65,65,65,65	0
56	MG	2a	1787	1/1	0.97	0.32	63,63,63,63	0
56	MG	1O	203	1/1	0.97	0.29	51,51,51,51	0
56	MG	1A	3653	1/1	0.97	0.17	24,24,24,24	0
56	MG	1A	3034	1/1	0.97	0.53	35,35,35,35	0
56	MG	1A	3701	1/1	0.97	0.11	44,44,44,44	0
56	MG	2A	3696	1/1	0.97	0.31	70,70,70,70	0
56	MG	1A	3393	1/1	0.97	0.26	59,59,59,59	0
56	MG	1A	3891	1/1	0.97	0.25	38,38,38,38	0
56	MG	1a	1827	1/1	0.97	0.17	70,70,70,70	0
56	MG	1A	3703	1/1	0.97	0.14	39,39,39,39	0
56	MG	2A	3057	1/1	0.97	0.10	71,71,71,71	0
56	MG	1A	3961	1/1	0.97	0.07	64,64,64,64	0
56	MG	2a	1632	1/1	0.97	0.11	87,87,87,87	0
56	MG	2A	3255	1/1	0.97	0.30	55,55,55,55	0
56	MG	1A	3229	1/1	0.97	0.23	51,51,51,51	0
56	MG	2a	1635	1/1	0.97	0.27	51,51,51,51	0
56	MG	1A	4033	1/1	0.97	0.18	24,24,24,24	0
56	MG	2A	3470	1/1	0.97	0.24	44,44,44,44	0
56	MG	1A	3069	1/1	0.97	0.19	27,27,27,27	0
56	MG	1A	3134	1/1	0.97	0.41	46,46,46,46	0
56	MG	1a	1685	1/1	0.97	0.22	44,44,44,44	0
56	MG	2A	3155	1/1	0.97	0.40	47,47,47,47	0
56	MG	1A	3897	1/1	0.97	0.20	40,40,40,40	0
56	MG	1A	3615	1/1	0.97	0.16	30,30,30,30	0
56	MG	1A	3276	1/1	0.97	0.17	47,47,47,47	0
56	MG	1A	4123	1/1	0.97	0.40	36,36,36,36	0
56	MG	1A	3399	1/1	0.97	0.32	51,51,51,51	0
56	MG	2A	3596	1/1	0.97	0.20	46,46,46,46	0
56	MG	1A	3210	1/1	0.97	0.52	32,32,32,32	0
56	MG	1A	3902	1/1	0.97	0.11	26,26,26,26	0
56	MG	1A	3021	1/1	0.97	0.18	21,21,21,21	0
56	MG	1A	3280	1/1	0.97	0.77	45,45,45,45	0
56	MG	2A	3165	1/1	0.97	0.05	38,38,38,38	0
56	MG	1l	203	1/1	0.97	0.10	49,49,49,49	0
56	MG	1A	4044	1/1	0.97	0.19	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	3714	1/1	0.97	0.15	46,46,46,46	0
56	MG	1A	4132	1/1	0.97	0.37	34,34,34,34	0
56	MG	1A	3136	1/1	0.97	0.06	36,36,36,36	0
56	MG	1A	3839	1/1	0.97	0.35	45,45,45,45	0
56	MG	2A	3171	1/1	0.97	0.12	55,55,55,55	0
56	MG	1X	104	1/1	0.97	0.99	43,43,43,43	0
56	MG	1a	1707	1/1	0.97	0.23	42,42,42,42	0
56	MG	2A	3077	1/1	0.97	0.09	44,44,44,44	0
56	MG	1A	3908	1/1	0.97	0.12	46,46,46,46	0
56	MG	1A	4136	1/1	0.97	0.17	31,31,31,31	0
56	MG	2a	1665	1/1	0.97	0.20	55,55,55,55	0
56	MG	1Y	203	1/1	0.97	1.12	57,57,57,57	0
56	MG	1A	3438	1/1	0.97	0.69	37,37,37,37	0
56	MG	2A	3495	1/1	0.97	0.18	51,51,51,51	0
56	MG	1w	107	1/1	0.97	0.09	38,38,38,38	0
56	MG	1A	4138	1/1	0.97	0.58	36,36,36,36	0
56	MG	1A	4051	1/1	0.97	0.18	11,11,11,11	0
56	MG	2A	3617	1/1	0.97	0.24	74,74,74,74	0
56	MG	2l	201	1/1	0.97	0.33	65,65,65,65	0
56	MG	2A	3179	1/1	0.97	0.09	46,46,46,46	0
56	MG	1A	4140	1/1	0.97	0.59	31,31,31,31	0
56	MG	2A	3737	1/1	0.97	0.06	41,41,41,41	0
56	MG	1x	107	1/1	0.97	0.21	54,54,54,54	0
56	MG	2a	1677	1/1	0.97	0.15	59,59,59,59	0
56	MG	10	106	1/1	0.97	0.09	44,44,44,44	0
56	MG	1A	4052	1/1	0.97	0.17	22,22,22,22	0
56	MG	1A	3172	1/1	0.97	0.88	40,40,40,40	0
56	MG	1A	3669	1/1	0.97	0.14	20,20,20,20	0
56	MG	11	103	1/1	0.97	0.34	67,67,67,67	0
56	MG	1y	101	1/1	0.97	0.47	34,34,34,34	0
56	MG	1a	1727	1/1	0.97	0.19	30,30,30,30	0
56	MG	1A	3174	1/1	0.97	0.21	37,37,37,37	0
56	MG	2x	105	1/1	0.97	0.12	56,56,56,56	0
56	MG	1a	1729	1/1	0.97	0.17	48,48,48,48	0
56	MG	1a	1730	1/1	0.97	0.16	55,55,55,55	0
56	MG	1A	3720	1/1	0.97	0.09	32,32,32,32	0
56	MG	1A	3721	1/1	0.97	0.07	30,30,30,30	0
56	MG	1A	4058	1/1	0.97	0.13	48,48,48,48	0
56	MG	1B	207	1/1	0.97	0.39	41,41,41,41	0
56	MG	2A	3628	1/1	0.97	0.12	55,55,55,55	0
56	MG	1A	3722	1/1	0.97	0.17	21,21,21,21	0
56	MG	1a	1737	1/1	0.97	0.13	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3724	1/1	0.97	0.21	76,76,76,76	0
56	MG	1A	3341	1/1	0.97	0.50	47,47,47,47	0
56	MG	1A	3547	1/1	0.97	0.92	38,38,38,38	0
56	MG	1A	3588	1/1	0.97	0.14	48,48,48,48	0
56	MG	1A	3062	1/1	0.97	0.16	53,53,53,53	0
56	MG	16	103	1/1	0.97	0.13	32,32,32,32	0
59	ZN	25	105	1/1	0.97	0.20	66,66,66,66	0
56	MG	1A	3343	1/1	0.97	0.61	38,38,38,38	0
56	MG	2A	3825	1/1	0.98	0.13	33,33,33,33	0
56	MG	2A	3584	1/1	0.98	0.16	33,33,33,33	0
56	MG	2A	3827	1/1	0.98	0.17	51,51,51,51	0
56	MG	1E	307	1/1	0.98	0.61	37,37,37,37	0
56	MG	1A	3097	1/1	0.98	0.21	34,34,34,34	0
56	MG	1A	4077	1/1	0.98	0.12	56,56,56,56	0
56	MG	1A	3383	1/1	0.98	0.16	43,43,43,43	0
56	MG	1A	3780	1/1	0.98	0.16	56,56,56,56	0
56	MG	1a	1799	1/1	0.98	0.10	36,36,36,36	0
56	MG	1A	3022	1/1	0.98	0.16	34,34,34,34	0
56	MG	1a	1696	1/1	0.98	0.25	39,39,39,39	0
56	MG	1A	3621	1/1	0.98	0.09	47,47,47,47	0
56	MG	1A	3828	1/1	0.98	0.07	56,56,56,56	0
56	MG	1A	3738	1/1	0.98	0.17	26,26,26,26	0
56	MG	1a	1601	1/1	0.98	0.22	51,51,51,51	0
56	MG	2A	3173	1/1	0.98	0.24	45,45,45,45	0
56	MG	1A	3784	1/1	0.98	0.18	16,16,16,16	0
56	MG	1A	3099	1/1	0.98	0.14	23,23,23,23	0
56	MG	1a	1704	1/1	0.98	0.11	62,62,62,62	0
56	MG	1A	3878	1/1	0.98	0.19	35,35,35,35	0
56	MG	2A	3375	1/1	0.98	0.07	47,47,47,47	0
56	MG	2a	1783	1/1	0.98	0.19	58,58,58,58	0
56	MG	2A	3521	1/1	0.98	0.42	53,53,53,53	0
56	MG	2A	3842	1/1	0.98	0.12	48,48,48,48	0
56	MG	1A	3879	1/1	0.98	0.15	40,40,40,40	0
56	MG	1A	3109	1/1	0.98	1.19	35,35,35,35	0
56	MG	1A	3137	1/1	0.98	0.55	40,40,40,40	0
56	MG	1A	3317	1/1	0.98	0.11	47,47,47,47	0
56	MG	2a	1790	1/1	0.98	0.13	58,58,58,58	0
56	MG	2a	1679	1/1	0.98	0.09	64,64,64,64	0
56	MG	1a	1713	1/1	0.98	0.29	58,58,58,58	0
56	MG	2A	3603	1/1	0.98	0.17	49,49,49,49	0
56	MG	2A	3181	1/1	0.98	0.13	63,63,63,63	0
56	MG	2A	3381	1/1	0.98	0.18	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	3110	1/1	0.98	0.51	29,29,29,29	0
56	MG	2A	3247	1/1	0.98	0.34	56,56,56,56	0
56	MG	1A	3559	1/1	0.98	0.39	34,34,34,34	0
56	MG	2A	3854	1/1	0.98	0.20	55,55,55,55	0
56	MG	1A	3986	1/1	0.98	0.08	21,21,21,21	0
56	MG	1A	3746	1/1	0.98	0.21	46,46,46,46	0
56	MG	2A	3611	1/1	0.98	0.12	48,48,48,48	0
56	MG	1a	1724	1/1	0.98	0.15	23,23,23,23	0
56	MG	1A	3560	1/1	0.98	0.54	42,42,42,42	0
56	MG	1A	3989	1/1	0.98	0.10	34,34,34,34	0
56	MG	1A	3887	1/1	0.98	0.09	31,31,31,31	0
56	MG	1a	1835	1/1	0.98	0.08	47,47,47,47	0
56	MG	1A	3082	1/1	0.98	0.43	35,35,35,35	0
56	MG	1A	3177	1/1	0.98	0.14	25,25,25,25	0
56	MG	1Q	202	1/1	0.98	0.55	37,37,37,37	0
56	MG	1A	4046	1/1	0.98	0.15	31,31,31,31	0
56	MG	2A	3618	1/1	0.98	0.12	30,30,30,30	0
56	MG	1A	3631	1/1	0.98	0.12	20,20,20,20	0
56	MG	1Q	206	1/1	0.98	0.16	25,25,25,25	0
56	MG	1A	3140	1/1	0.98	0.38	34,34,34,34	0
56	MG	1A	3141	1/1	0.98	0.16	17,17,17,17	0
56	MG	1A	3421	1/1	0.98	0.23	40,40,40,40	0
56	MG	1A	3845	1/1	0.98	0.16	28,28,28,28	0
56	MG	1A	3300	1/1	0.98	0.23	32,32,32,32	0
56	MG	1f	201	1/1	0.98	0.18	46,46,46,46	0
56	MG	1A	3112	1/1	0.98	0.39	37,37,37,37	0
56	MG	1A	3637	1/1	0.98	0.11	12,12,12,12	0
56	MG	1A	3568	1/1	0.98	0.71	31,31,31,31	0
56	MG	1a	1743	1/1	0.98	0.15	49,49,49,49	0
56	MG	1A	4111	1/1	0.98	0.48	32,32,32,32	0
56	MG	1A	3200	1/1	0.98	0.18	37,37,37,37	0
56	MG	2A	3203	1/1	0.98	0.18	35,35,35,35	0
56	MG	2A	3551	1/1	0.98	0.16	59,59,59,59	0
56	MG	1A	3506	1/1	0.98	0.53	26,26,26,26	0
56	MG	2A	3335	1/1	0.98	0.31	61,61,61,61	0
56	MG	1a	1647	1/1	0.98	0.11	35,35,35,35	0
56	MG	2A	3554	1/1	0.98	0.13	46,46,46,46	0
56	MG	1a	1649	1/1	0.98	0.10	54,54,54,54	0
56	MG	2A	3337	1/1	0.98	0.32	37,37,37,37	0
56	MG	1a	1754	1/1	0.98	0.10	58,58,58,58	0
56	MG	1A	3037	1/1	0.98	0.15	22,22,22,22	0
56	MG	2A	3206	1/1	0.98	0.17	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1a	1653	1/1	0.98	0.29	50,50,50,50	0
56	MG	1B	222	1/1	0.98	0.20	51,51,51,51	0
56	MG	1A	3761	1/1	0.98	0.11	43,43,43,43	0
56	MG	1A	4116	1/1	0.98	0.50	33,33,33,33	0
56	MG	1W	206	1/1	0.98	0.51	31,31,31,31	0
56	MG	1A	4117	1/1	0.98	0.42	29,29,29,29	0
56	MG	2A	3562	1/1	0.98	0.08	43,43,43,43	0
56	MG	1A	3032	1/1	0.98	0.73	32,32,32,32	0
56	MG	1A	3374	1/1	0.98	0.35	43,43,43,43	0
56	MG	2A	3088	1/1	0.98	0.41	48,48,48,48	0
56	MG	2v	101	1/1	0.98	0.16	54,54,54,54	0
56	MG	1A	3644	1/1	0.98	0.06	35,35,35,35	0
56	MG	1A	3128	1/1	0.98	0.38	30,30,30,30	0
56	MG	1A	3284	1/1	0.98	0.33	45,45,45,45	0
56	MG	2A	3491	1/1	0.98	0.12	51,51,51,51	0
56	MG	2A	3032	1/1	0.98	0.27	36,36,36,36	0
56	MG	1A	3430	1/1	0.98	0.85	41,41,41,41	0
56	MG	1A	3014	1/1	0.98	0.16	29,29,29,29	0
56	MG	1A	3726	1/1	0.98	0.20	65,65,65,65	0
56	MG	1A	3024	1/1	0.98	0.49	33,33,33,33	0
56	MG	1D	302	1/1	0.98	0.18	33,33,33,33	0
56	MG	2a	1747	1/1	0.98	0.18	51,51,51,51	0
56	MG	2A	3037	1/1	0.98	0.26	35,35,35,35	0
56	MG	1D	304	1/1	0.98	0.44	36,36,36,36	0
56	MG	1A	3515	1/1	0.98	0.14	75,75,75,75	0
56	MG	1a	1676	1/1	0.98	0.20	35,35,35,35	0
56	MG	1A	3729	1/1	0.98	0.11	44,44,44,44	0
56	MG	1A	3131	1/1	0.98	0.20	62,62,62,62	0
56	MG	1D	309	1/1	0.98	0.35	27,27,27,27	0
56	MG	1A	3581	1/1	0.98	0.43	42,42,42,42	0
56	MG	1A	3012	1/1	0.98	0.13	23,23,23,23	0
56	MG	2B	211	1/1	0.98	0.10	61,61,61,61	0
59	ZN	16	102	1/1	0.98	0.21	38,38,38,38	0
56	MG	2A	3430	1/1	0.98	0.08	40,40,40,40	0
56	MG	1A	3227	1/1	0.98	0.12	34,34,34,34	0
56	MG	1A	3919	1/1	0.98	0.08	44,44,44,44	0
59	ZN	26	501	1/1	0.98	0.21	58,58,58,58	0
56	MG	2A	3744	1/1	0.98	0.15	35,35,35,35	0
60	SF4	1d	3102	8/8	0.98	0.18	47,58,62,63	0
60	SF4	2d	303	8/8	0.98	0.17	62,72,82,88	0
56	MG	1A	3664	1/1	0.99	0.09	39,39,39,39	0
56	MG	1A	3144	1/1	0.99	0.27	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	1a	1678	1/1	0.99	0.28	35,35,35,35	0
56	MG	2A	3517	1/1	0.99	0.13	17,17,17,17	0
56	MG	2A	3645	1/1	0.99	0.18	55,55,55,55	0
56	MG	1A	3527	1/1	0.99	0.25	37,37,37,37	0
56	MG	1A	4128	1/1	0.99	0.23	30,30,30,30	0
56	MG	1A	3278	1/1	0.99	0.66	27,27,27,27	0
56	MG	1A	3058	1/1	0.99	0.11	27,27,27,27	0
56	MG	1A	3707	1/1	0.99	0.09	16,16,16,16	0
56	MG	2A	3717	1/1	0.99	0.08	69,69,69,69	0
56	MG	1A	3614	1/1	0.99	0.17	31,31,31,31	0
56	MG	1A	3530	1/1	0.99	0.13	33,33,33,33	0
56	MG	1A	3094	1/1	0.99	0.14	17,17,17,17	0
56	MG	2A	3464	1/1	0.99	0.20	31,31,31,31	0
56	MG	1A	3774	1/1	0.99	0.15	34,34,34,34	0
56	MG	2a	1689	1/1	0.99	0.12	52,52,52,52	0
56	MG	2A	3559	1/1	0.99	0.13	32,32,32,32	0
56	MG	1A	3192	1/1	0.99	0.60	23,23,23,23	0
56	MG	2A	3467	1/1	0.99	0.28	29,29,29,29	0
56	MG	1A	3073	1/1	0.99	0.16	30,30,30,30	0
56	MG	1A	3173	1/1	0.99	0.53	34,34,34,34	0
56	MG	1A	3800	1/1	0.99	0.12	43,43,43,43	0
56	MG	1A	3893	1/1	0.99	0.11	48,48,48,48	0
56	MG	1A	3126	1/1	0.99	0.20	32,32,32,32	0
56	MG	1A	3552	1/1	0.99	0.19	33,33,33,33	0
56	MG	1A	3077	1/1	0.99	0.24	39,39,39,39	0
56	MG	1A	3395	1/1	0.99	0.13	33,33,33,33	0
56	MG	1D	306	1/1	0.99	0.14	23,23,23,23	0
56	MG	1A	3739	1/1	0.99	0.18	35,35,35,35	0
56	MG	1a	1817	1/1	0.99	0.13	54,54,54,54	0
56	MG	1A	3086	1/1	0.99	0.10	34,34,34,34	0
56	MG	1a	1819	1/1	0.99	0.13	37,37,37,37	0
59	ZN	15	106	1/1	0.99	0.19	42,42,42,42	0
56	MG	2A	3336	1/1	0.99	0.33	50,50,50,50	0
59	ZN	19	501	1/1	0.99	0.23	57,57,57,57	0
59	ZN	1n	101	1/1	0.99	0.16	49,49,49,49	0
56	MG	1A	3031	1/1	0.99	0.45	32,32,32,32	0
56	MG	1A	3168	1/1	0.99	0.56	34,34,34,34	0
56	MG	1A	4022	1/1	0.99	0.13	17,17,17,17	0
56	MG	1D	313	1/1	0.99	0.56	39,39,39,39	0
59	ZN	29	501	1/1	0.99	0.13	65,65,65,65	0
56	MG	1a	1785	1/1	0.99	0.12	64,64,64,64	0
56	MG	1A	3385	1/1	0.99	0.30	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	3341	1/1	0.99	0.20	73,73,73,73	0
56	MG	1A	3723	1/1	1.00	0.17	14,14,14,14	0

6.5 Other polymers (i)

There are no such residues in this entry.