Full wwPDB X-ray Structure Validation Report ⓘ

Nov 7, 2023 – 07:50 AM EST

PDB ID	:	7JQL
Title	:	Crystal structure of the Thermus thermophilus 70S ribosome in complex with Bac7-001, mRNA, and deacylated P-site tRNA at 3.00A resolution
Authors	:	Mardirossian, M.; Sola, R.; Beckert, B.; Valencic, E.; Collis, D.W.P.; Borisek, J.; Armas, F.; Di Stasi, A.; Buchmann, J.; Syroegin, E.A.; Polikanov, Y.S.; Magistrato, A.; Hilpert, K.; Wilson, D.N.; Scocchi, M.
Deposited on	:	2020-08-11
Resolution	:	3.00 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:

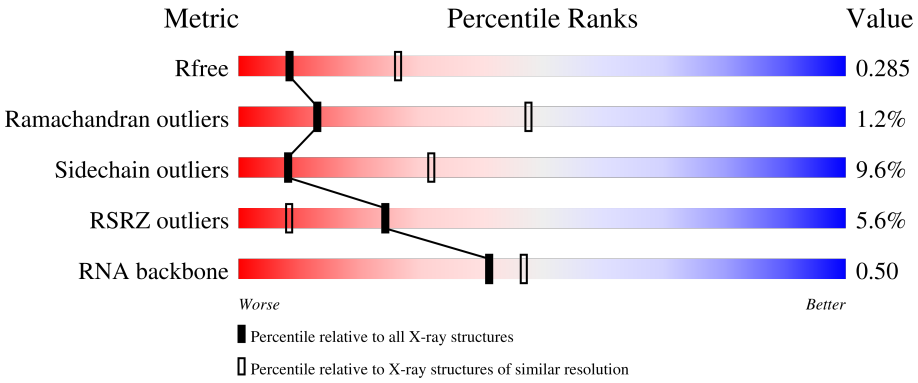
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

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	80% 18%
1	2A	2915	77% 19%
2	1B	121	87% 12%
2	2B	121	71% 28%

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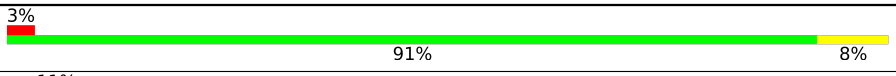
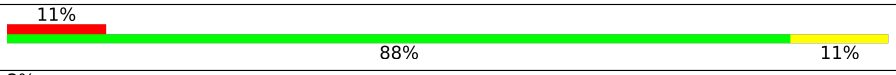
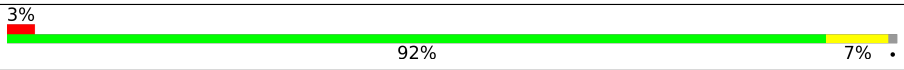
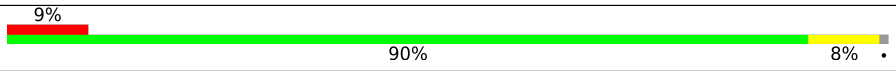
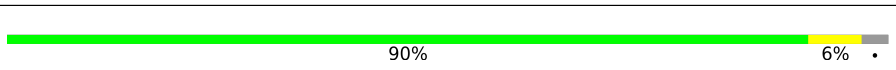
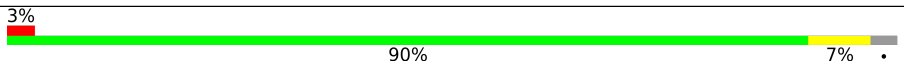
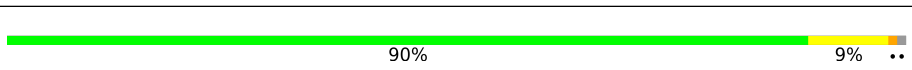
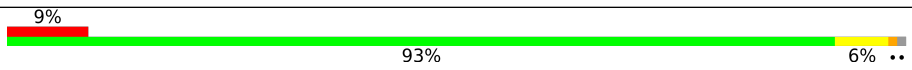
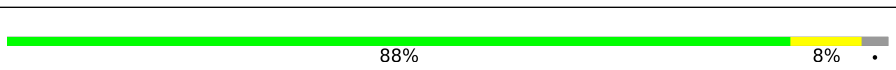
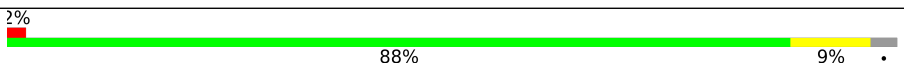
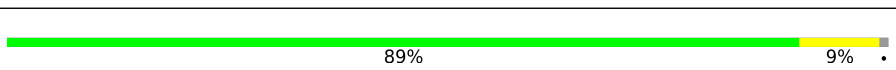
Mol	Chain	Length	Quality of chain
3	1D	276	
3	2D	276	
4	1E	206	
4	2E	206	
5	1F	210	
5	2F	210	
6	1G	182	
6	2G	182	
7	1H	180	
7	2H	180	
8	1I	148	
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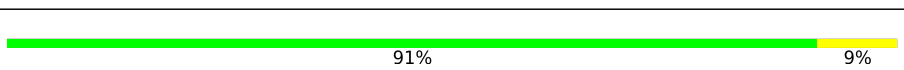
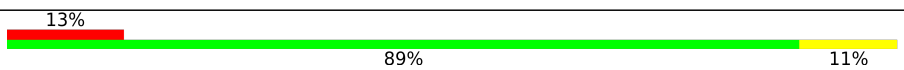
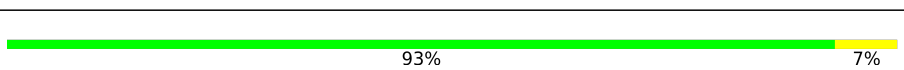
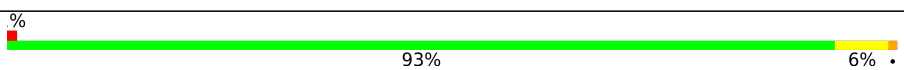
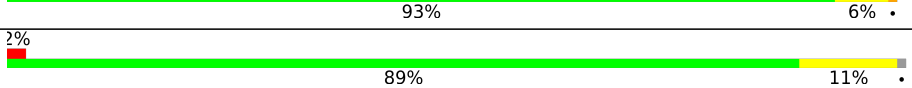
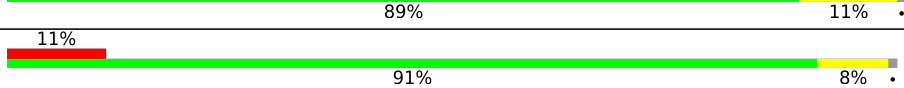
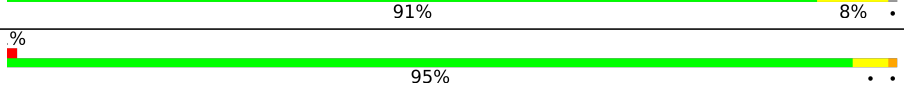
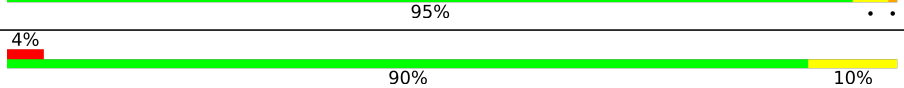
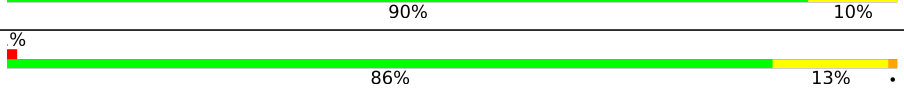
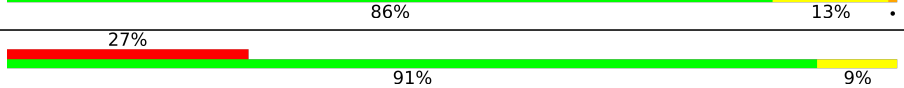
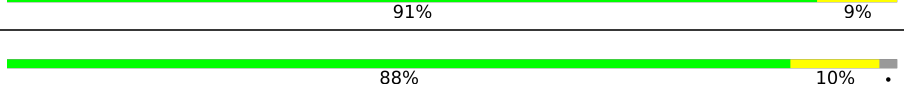
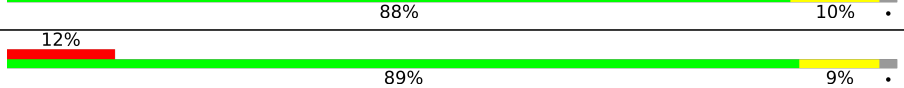
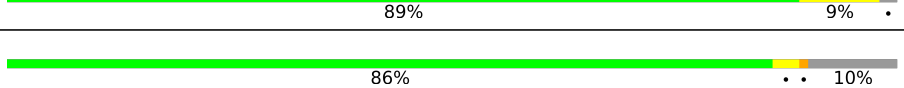
9	1N	140	
9	2N	140	
10	1O	122	
10	2O	122	
11	1P	150	
11	2P	150	
12	1Q	141	
12	2Q	141	
13	1R	118	
13	2R	118	
14	1S	112	
14	2S	112	
15	1T	146	

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Mol	Chain	Length	Quality of chain
15	2T	146	4% 83% 7% 10%
16	1U	118	3% 92% 7%
16	2U	118	3% 92% 6%
17	1V	101	90% 10%
17	2V	101	3% 94% 5%
18	1W	113	93% 6%
18	2W	113	3% 95%
19	1X	96	% 95%
19	2X	96	5% 95%
20	1Y	110	% 88% 9%
20	2Y	110	14% 86% 11%
21	1Z	206	68% 6% 25%
21	2Z	206	65% 13% 22%
22	10	85	86% 11%
22	20	85	36% 82% 7% 11%
23	11	98	3% 96%
23	21	98	17% 95%
24	12	72	89% 8%
24	22	72	4% 90% 7%
25	13	60	88% 10%
25	23	60	10% 93% 5%
26	14	71	82% 14%
26	24	71	6% 85% 13%
27	15	60	88% 10%
27	25	60	2% 92% 5%

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Mol	Chain	Length	Quality of chain
28	16	54	2% 83% 15%
28	26	54	81% 17%
29	17	49	10% 90% 8%
29	27	49	16% 82% 16%
30	18	65	12% 92% 6%
30	28	65	25% 91% 8%
31	19	37	16% 95% 5%
31	29	37	38% 89% 11%
32	1a	1521	4% 79% 19%
32	2a	1521	6% 80% 18%
33	1b	256	79% 11% 10%
33	2b	256	3% 77% 12% 10%
34	1c	239	6% 80% 6% 14%
34	2c	239	5% 75% 11% 14%
35	1d	209	12% 90% 10%
35	2d	209	2% 93% 7%
36	1e	162	6% 83% 9% 9%
36	2e	162	7% 84% 7% 9%
37	1f	101	91% 8%
37	2f	101	88% 11%
38	1g	156	4% 94% 5%
38	2g	156	10% 91% 8%
39	1h	138	9% 92% 7%
39	2h	138	17% 94% 5%
40	1i	128	22% 87% 12%

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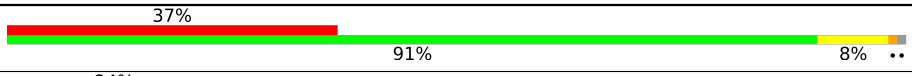
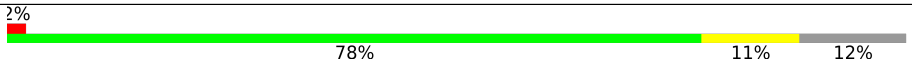
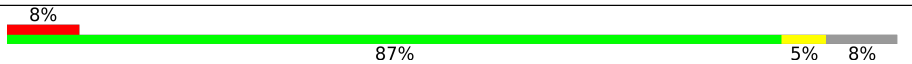
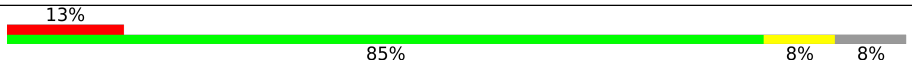
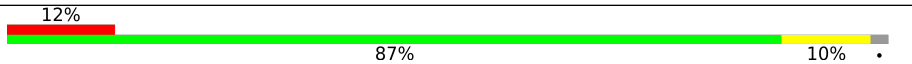
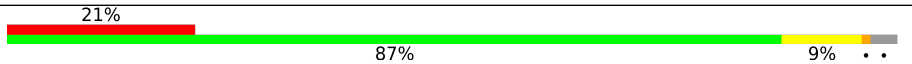
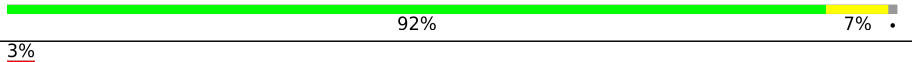
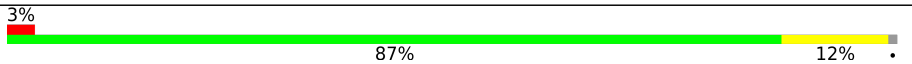
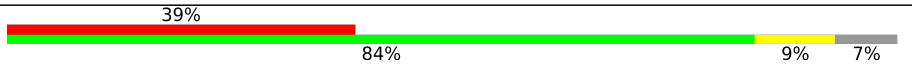
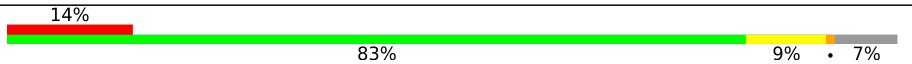
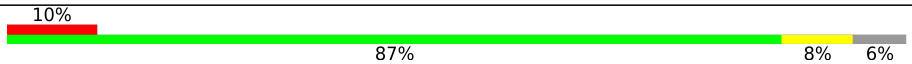
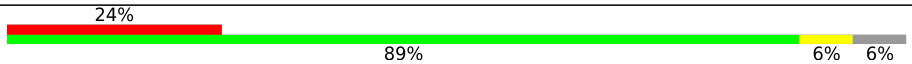
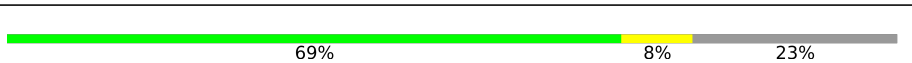
Mol	Chain	Length	Quality of chain
40	2i	128	
41	1j	105	
41	2j	105	
42	1k	129	
42	2k	129	
43	1l	132	
43	2l	132	
44	1m	126	
44	2m	126	
45	1n	61	
45	2n	61	
46	1o	89	
46	2o	89	
47	1p	88	
47	2p	88	
48	1q	105	
48	2q	105	
49	1r	88	
49	2r	88	
50	1s	93	
50	2s	93	
51	1t	106	
51	2t	106	
52	1u	27	
52	2u	27	

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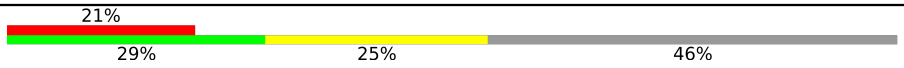
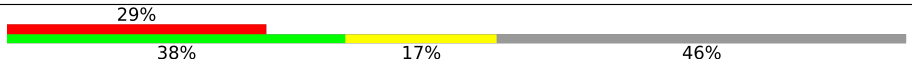
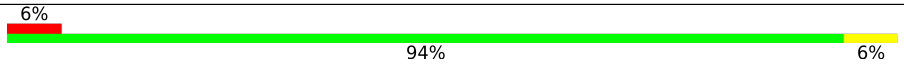
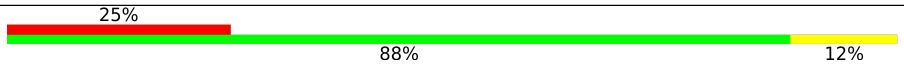
Mol	Chain	Length	Quality of chain
53	1v	24	
53	2v	24	
54	1x	77	
54	2x	77	
55	1z	16	
55	2z	16	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1A	3050	-	-	-	X
56	MG	1A	3313	-	-	-	X
56	MG	1A	3390	-	-	-	X
56	MG	1A	3440	-	-	-	X
56	MG	1A	3465	-	-	-	X
56	MG	1A	3487	-	-	-	X
56	MG	1A	3857	-	-	-	X
56	MG	1A	3925	-	-	-	X
56	MG	1A	3936	-	-	-	X
56	MG	1A	3962	-	-	-	X
56	MG	1A	4041	-	-	-	X
56	MG	1P	204	-	-	-	X
56	MG	1a	1660	-	-	-	X
56	MG	2A	3022	-	-	-	X
56	MG	2A	3030	-	-	-	X
56	MG	2A	3066	-	-	-	X
56	MG	2A	3069	-	-	-	X
56	MG	2A	3080	-	-	-	X
56	MG	2A	3184	-	-	-	X
56	MG	2A	3209	-	-	-	X
56	MG	2A	3222	-	-	-	X
56	MG	2A	3263	-	-	-	X
56	MG	2A	3277	-	-	-	X
56	MG	2A	3292	-	-	-	X
56	MG	2A	3319	-	-	-	X
56	MG	2A	3332	-	-	-	X
56	MG	2A	3468	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	2A	3716	-	-	-	X
56	MG	2a	3022	-	-	-	X
56	MG	2a	3109	-	-	-	X
56	MG	2a	3171	-	-	-	X

2 Entry composition (i)

There are 60 unique types of molecules in this entry. The entry contains 293228 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	76	Total	C	N	O	S	0	0	0
			604	373	128	102	1			
22	20	76	Total	C	N	O	S	0	0	0
			604	373	128	102	1			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 53 is a RNA chain called mRNA.

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

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

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

- Molecule 55 is a protein called Bac7-001.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
55	1z	16	Total	C	N	O	0	0	0
			143	92	35	16			
55	2z	16	Total	C	N	O	0	0	0
			143	92	35	16			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1A	1041	Total	Mg	0	0
			1041	1041		
56	1B	31	Total	Mg	0	0
			31	31		
56	1D	10	Total	Mg	0	0
			10	10		
56	1E	9	Total	Mg	0	0
			9	9		
56	1F	9	Total	Mg	0	0
			9	9		
56	1G	4	Total	Mg	0	0
			4	4		
56	1N	2	Total	Mg	0	0
			2	2		
56	1O	2	Total	Mg	0	0
			2	2		
56	1P	4	Total	Mg	0	0
			4	4		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	1Q	5	Total Mg 5 5	0	0
56	1R	3	Total Mg 3 3	0	0
56	1S	2	Total Mg 2 2	0	0
56	1T	5	Total Mg 5 5	0	0
56	1U	10	Total Mg 10 10	0	0
56	1V	6	Total Mg 6 6	0	0
56	1W	5	Total Mg 5 5	0	0
56	1X	5	Total Mg 5 5	0	0
56	1Y	1	Total Mg 1 1	0	0
56	1Z	2	Total Mg 2 2	0	0
56	10	8	Total Mg 8 8	0	0
56	11	1	Total Mg 1 1	0	0
56	13	4	Total Mg 4 4	0	0
56	15	7	Total Mg 7 7	0	0
56	16	2	Total Mg 2 2	0	0
56	17	7	Total Mg 7 7	0	0
56	18	3	Total Mg 3 3	0	0
56	19	2	Total Mg 2 2	0	0
56	1a	221	Total Mg 221 221	0	0
56	1b	1	Total Mg 1 1	0	0
56	1e	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	1f	2	Total Mg 2 2	0	0
56	1h	1	Total Mg 1 1	0	0
56	1l	3	Total Mg 3 3	0	0
56	1m	1	Total Mg 1 1	0	0
56	1n	2	Total Mg 2 2	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	1x	15	Total Mg 15 15	0	0
56	2A	810	Total Mg 810 810	0	0
56	2B	15	Total Mg 15 15	0	0
56	2D	4	Total Mg 4 4	0	0
56	2E	9	Total Mg 9 9	0	0
56	2F	2	Total Mg 2 2	0	0
56	2G	1	Total Mg 1 1	0	0
56	2O	2	Total Mg 2 2	0	0
56	2P	2	Total Mg 2 2	0	0
56	2Q	2	Total Mg 2 2	0	0
56	2R	4	Total Mg 4 4	0	0
56	2T	4	Total Mg 4 4	0	0
56	2U	2	Total Mg 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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	2Y	1	Total Mg 1 1	0	0
56	20	3	Total Mg 3 3	0	0
56	23	1	Total Mg 1 1	0	0
56	25	4	Total Mg 4 4	0	0
56	26	1	Total Mg 1 1	0	0
56	27	1	Total Mg 1 1	0	0
56	28	1	Total Mg 1 1	0	0
56	2a	217	Total Mg 217 217	0	0
56	2d	1	Total Mg 1 1	0	0
56	2e	1	Total Mg 1 1	0	0
56	2f	1	Total Mg 1 1	0	0
56	2i	1	Total Mg 1 1	0	0
56	2k	1	Total Mg 1 1	0	0
56	2l	1	Total Mg 1 1	0	0
56	2n	1	Total Mg 1 1	0	0
56	2q	1	Total Mg 1 1	0	0
56	2r	1	Total Mg 1 1	0	0
56	2t	1	Total Mg 1 1	0	0

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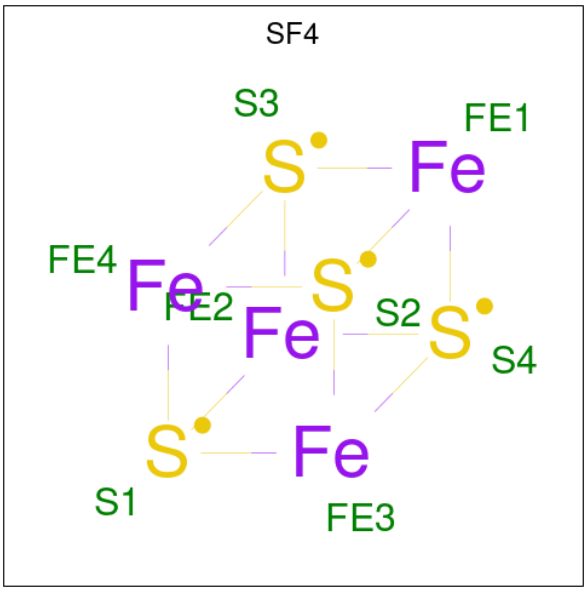
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	2v	1	Total Mg 1 1	0	0
56	2x	5	Total Mg 5 5	0	0

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

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

- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

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

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

- Molecule 60 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	1A	1949	Total O 1949 1949	0	0
60	1B	50	Total O 50 50	0	0
60	1D	21	Total O 21 21	0	0
60	1E	14	Total O 14 14	0	0
60	1F	9	Total O 9 9	0	0
60	1G	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	1N	3	Total O 3 3	0	0
60	1O	4	Total O 4 4	0	0
60	1P	17	Total O 17 17	0	0
60	1Q	3	Total O 3 3	0	0
60	1R	8	Total O 8 8	0	0
60	1S	1	Total O 1 1	0	0
60	1T	3	Total O 3 3	0	0
60	1U	5	Total O 5 5	0	0
60	1V	2	Total O 2 2	0	0
60	1W	5	Total O 5 5	0	0
60	1X	3	Total O 3 3	0	0
60	1Y	1	Total O 1 1	0	0
60	10	5	Total O 5 5	0	0
60	11	6	Total O 6 6	0	0
60	13	5	Total O 5 5	0	0
60	14	1	Total O 1 1	0	0
60	15	5	Total O 5 5	0	0
60	16	1	Total O 1 1	0	0
60	17	7	Total O 7 7	0	0
60	18	12	Total O 12 12	0	0
60	19	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	1a	301	Total O 301 301	0	0
60	1b	1	Total O 1 1	0	0
60	1e	1	Total O 1 1	0	0
60	1i	1	Total O 1 1	0	0
60	1l	4	Total O 4 4	0	0
60	1o	1	Total O 1 1	0	0
60	1q	3	Total O 3 3	0	0
60	1v	5	Total O 5 5	0	0
60	1x	16	Total O 16 16	0	0
60	1z	3	Total O 3 3	0	0
60	2A	917	Total O 917 917	0	0
60	2B	4	Total O 4 4	0	0
60	2D	14	Total O 14 14	0	0
60	2E	10	Total O 10 10	0	0
60	2F	12	Total O 12 12	0	0
60	2N	1	Total O 1 1	0	0
60	2O	2	Total O 2 2	0	0
60	2P	8	Total O 8 8	0	0
60	2Q	1	Total O 1 1	0	0
60	2R	2	Total O 2 2	0	0
60	2T	2	Total O 2 2	0	0

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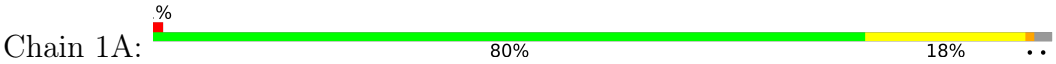
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	2U	2	Total O 2 2	0	0
60	2X	2	Total O 2 2	0	0
60	21	7	Total O 7 7	0	0
60	27	1	Total O 1 1	0	0
60	28	3	Total O 3 3	0	0
60	2a	286	Total O 286 286	0	0
60	2d	1	Total O 1 1	0	0
60	2e	3	Total O 3 3	0	0
60	2i	1	Total O 1 1	0	0
60	2l	2	Total O 2 2	0	0
60	2p	1	Total O 1 1	0	0
60	2r	1	Total O 1 1	0	0
60	2t	1	Total O 1 1	0	0
60	2v	2	Total O 2 2	0	0

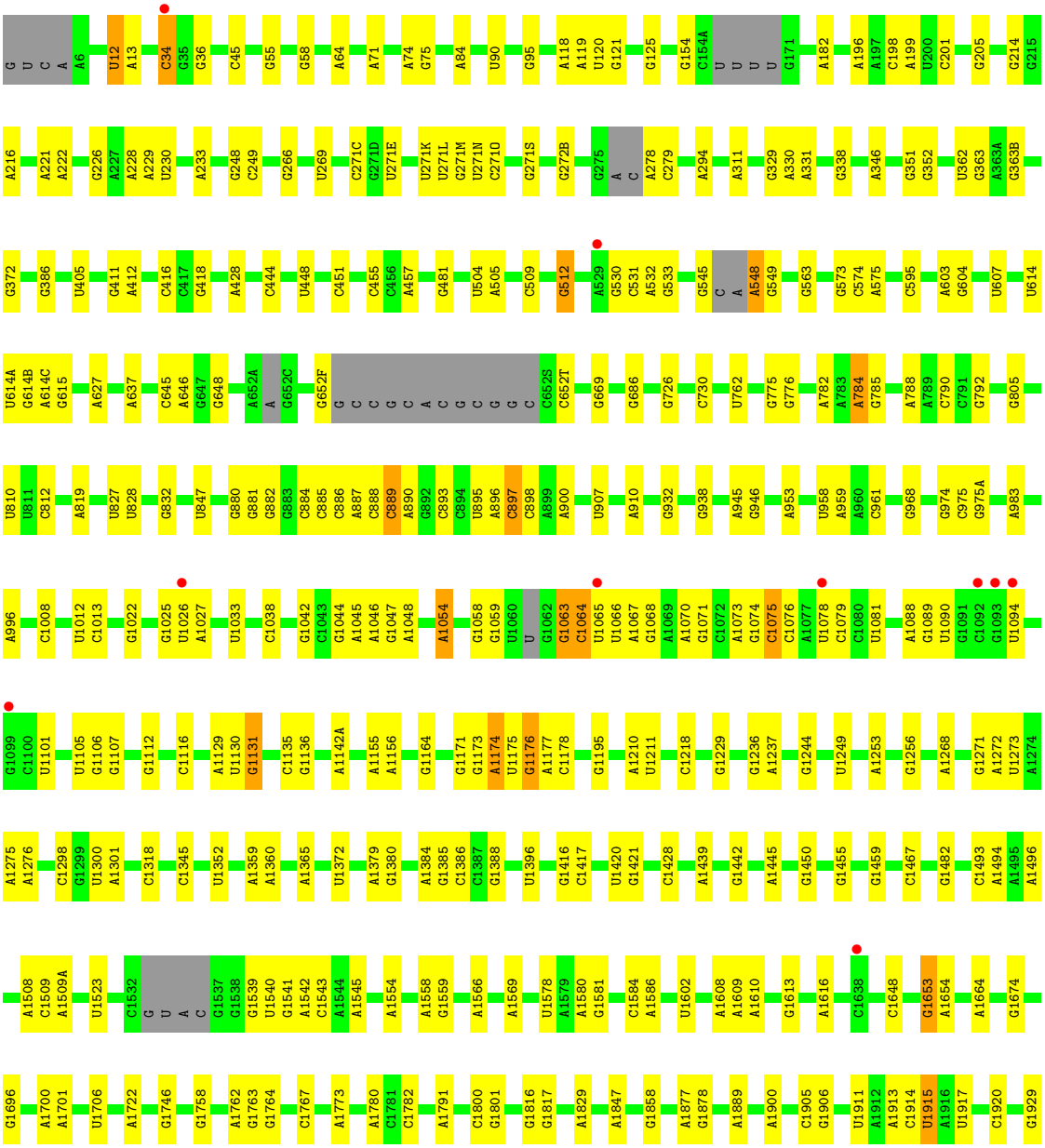
3 Residue-property plots (i)

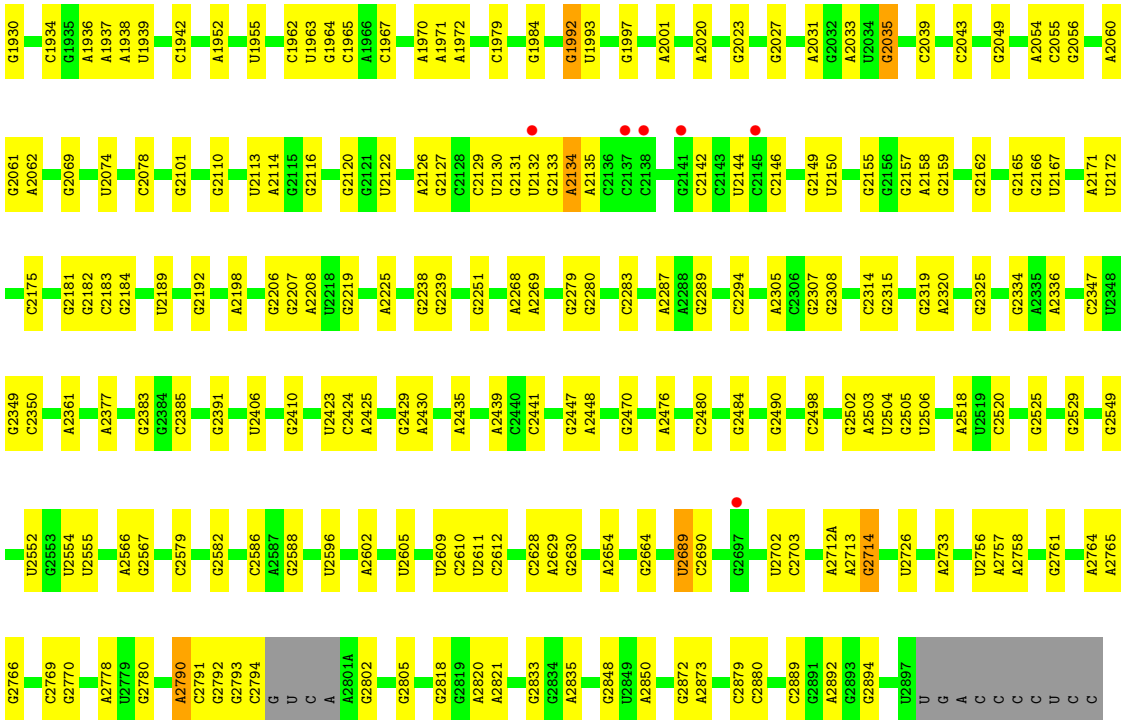
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: 23S Ribosomal RNA

Chain 1A:

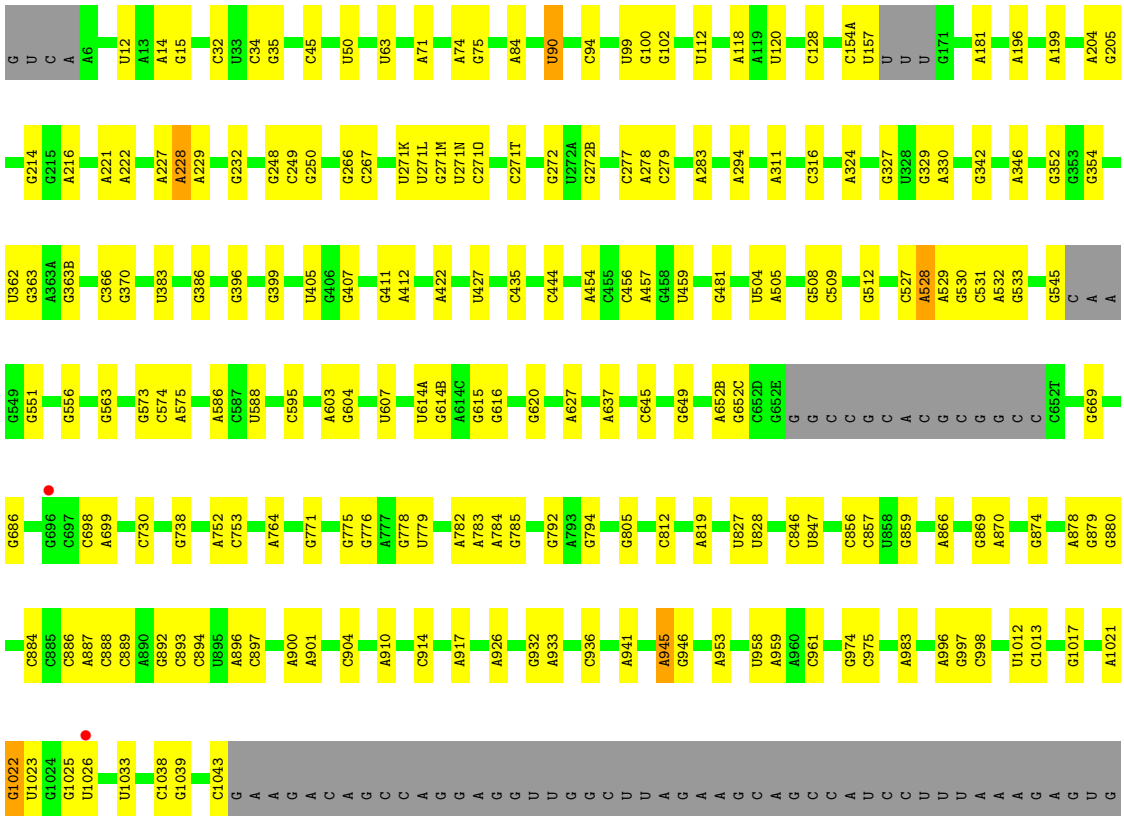


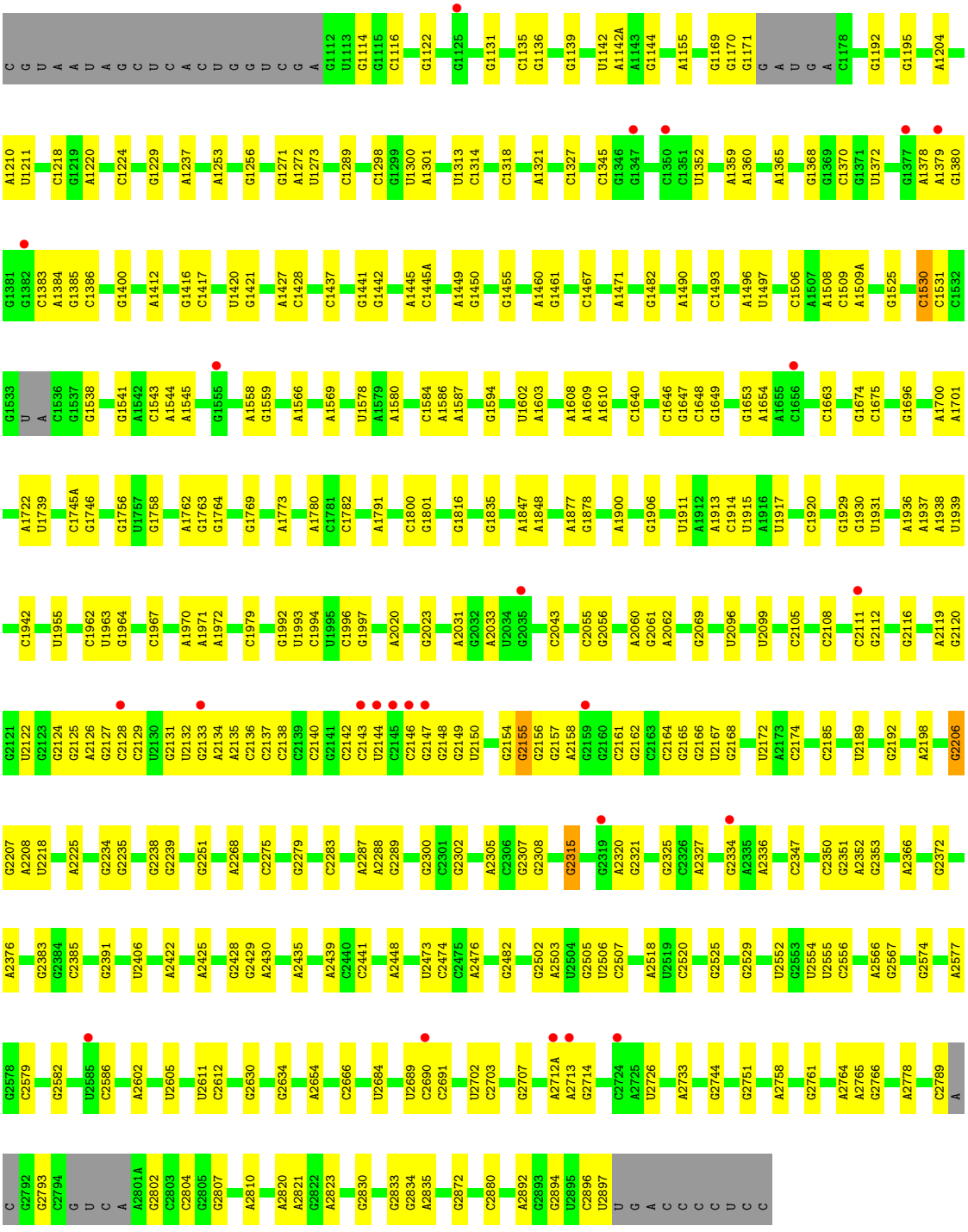




• Molecule 1: 23S Ribosomal RNA

Chain 2A:



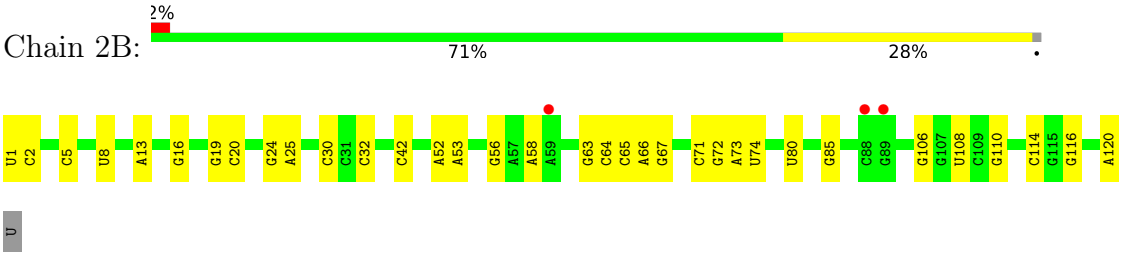


• Molecule 2: 5S Ribosomal RNA

Chain 1B:

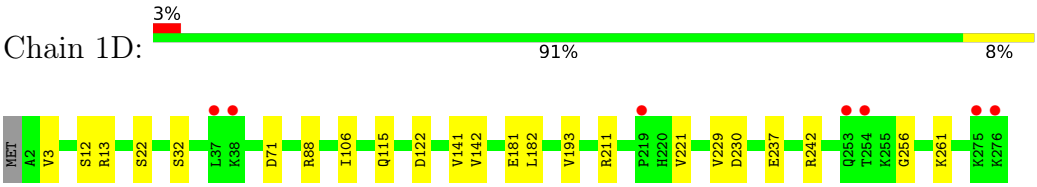
• Molecule 2: 5S Ribosomal RNA

Chain 2B:



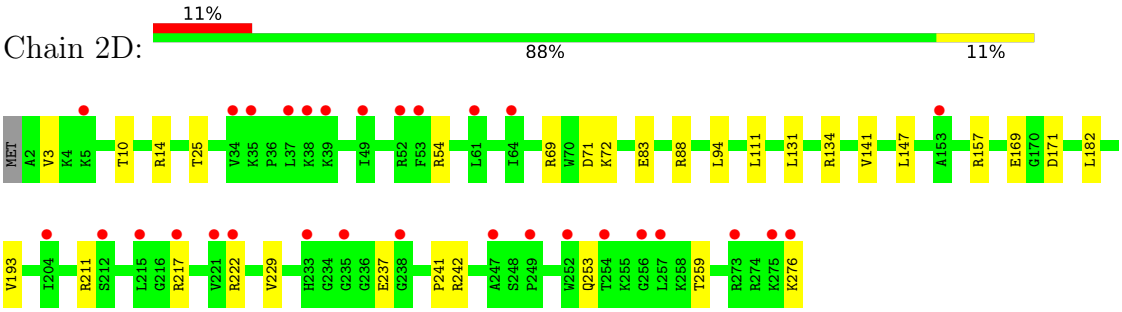
• Molecule 3: 50S ribosomal protein L2

Chain 1D:



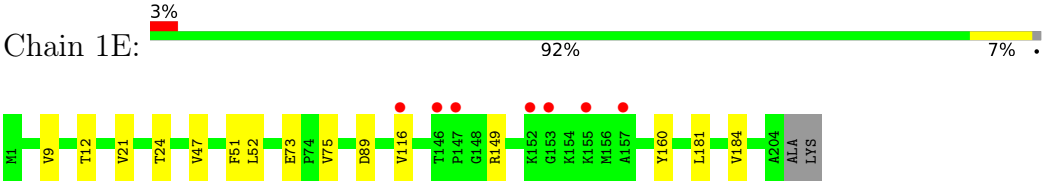
• Molecule 3: 50S ribosomal protein L2

Chain 2D:



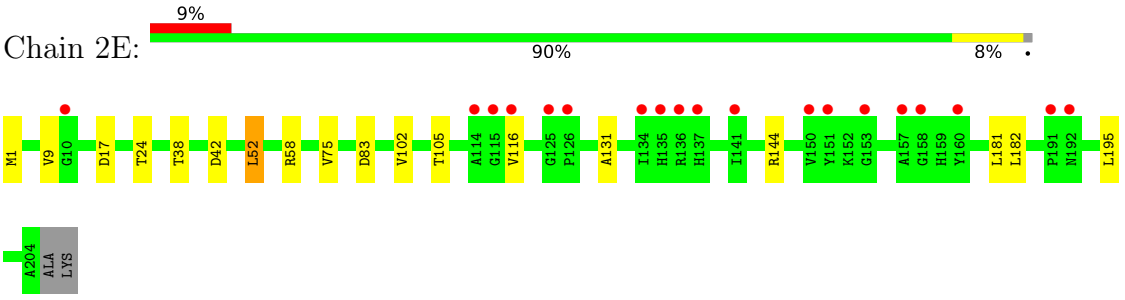
• Molecule 4: 50S ribosomal protein L3

Chain 1E:



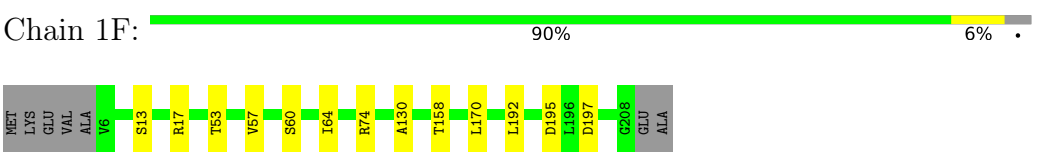
• Molecule 4: 50S ribosomal protein L3

Chain 2E:



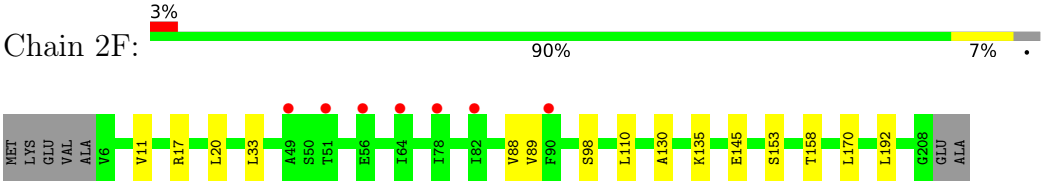
• Molecule 5: 50S ribosomal protein L4

Chain 1F:



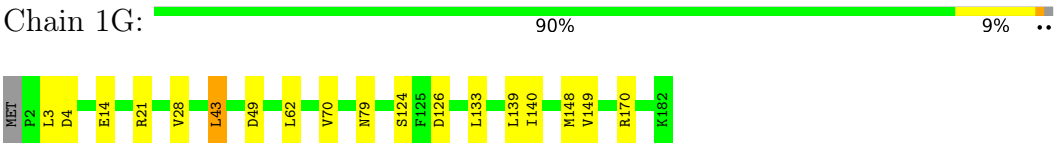
• Molecule 5: 50S ribosomal protein L4

Chain 2F:



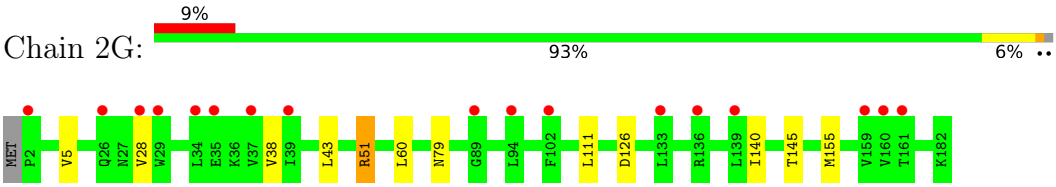
• Molecule 6: 50S ribosomal protein L5

Chain 1G:



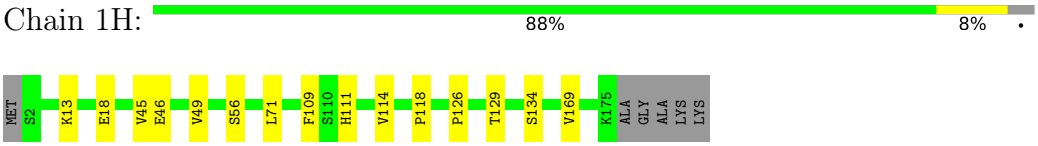
• Molecule 6: 50S ribosomal protein L5

Chain 2G:



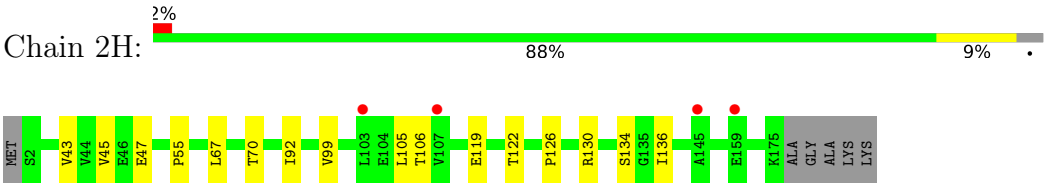
• Molecule 7: 50S ribosomal protein L6

Chain 1H:



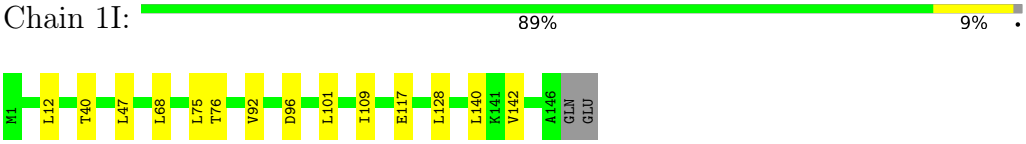
• Molecule 7: 50S ribosomal protein L6

Chain 2H:



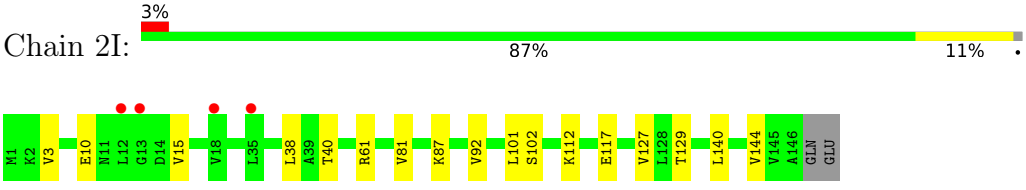
• Molecule 8: 50S ribosomal protein L9

Chain 1I:



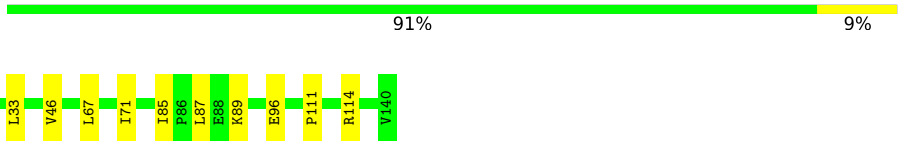
• Molecule 8: 50S ribosomal protein L9

Chain 2I:



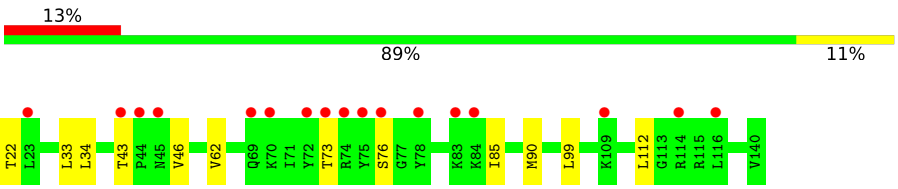
• Molecule 9: 50S ribosomal protein L13

Chain 1N:



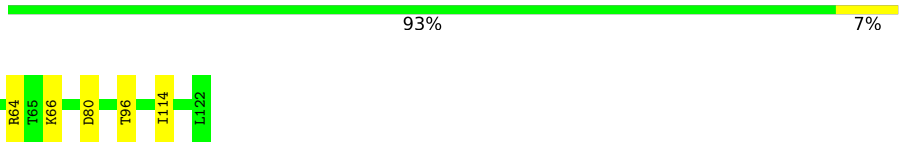
• Molecule 9: 50S ribosomal protein L13

Chain 2N:



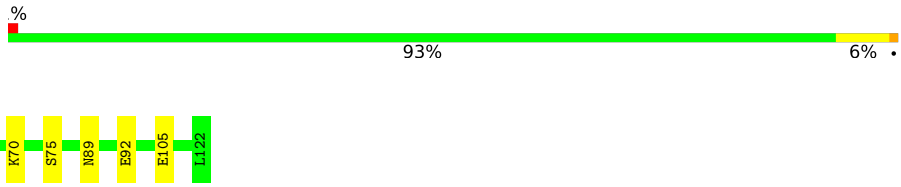
• Molecule 10: 50S ribosomal protein L14

Chain 1O:



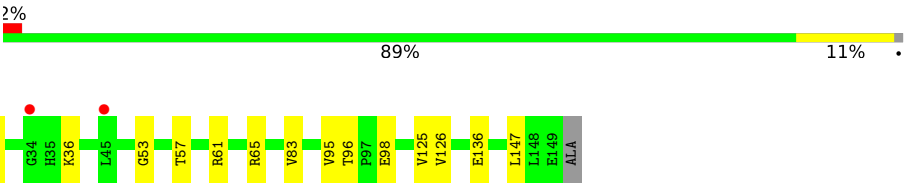
• Molecule 10: 50S ribosomal protein L14

Chain 2O:



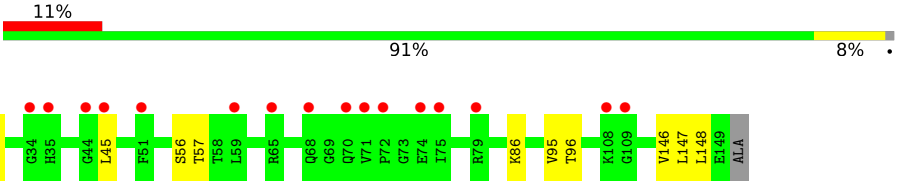
• Molecule 11: 50S ribosomal protein L15

Chain 1P:



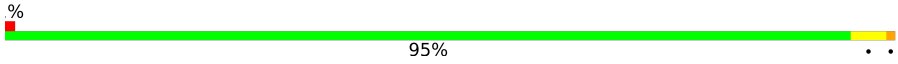
• Molecule 11: 50S ribosomal protein L15

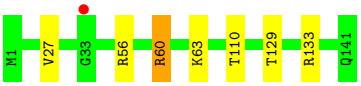
Chain 2P:



• Molecule 12: 50S ribosomal protein L16

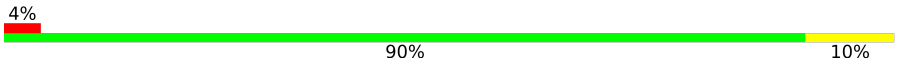
Chain 1Q:





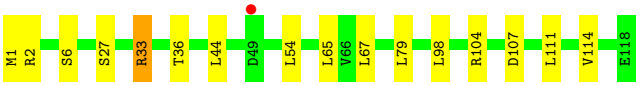
• Molecule 12: 50S ribosomal protein L16

Chain 2Q:



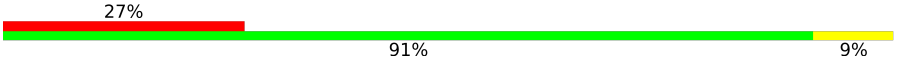
• Molecule 13: 50S ribosomal protein L17

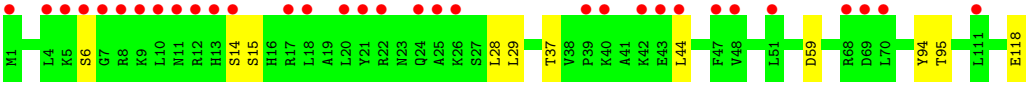
Chain 1R:



• Molecule 13: 50S ribosomal protein L17

Chain 2R:



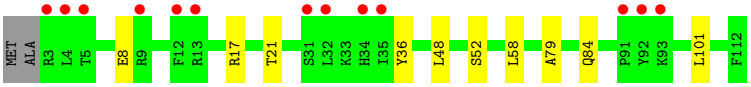


• Molecule 14: 50S ribosomal protein L18

Chain 1S:

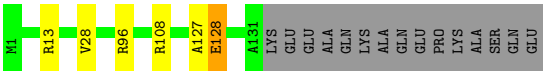
• Molecule 14: 50S ribosomal protein L18

Chain 2S:



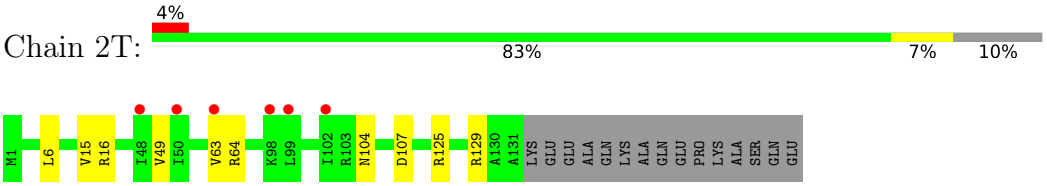
• Molecule 15: 50S ribosomal protein L19

Chain 1T:



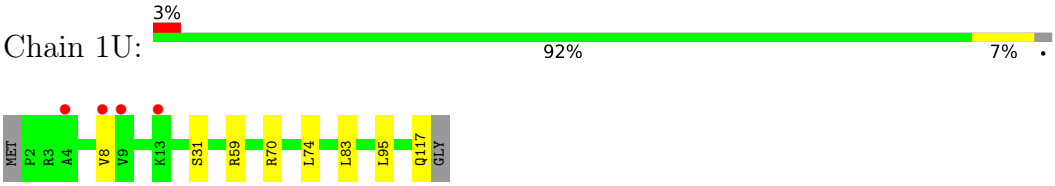
• Molecule 15: 50S ribosomal protein L19

Chain 2T:



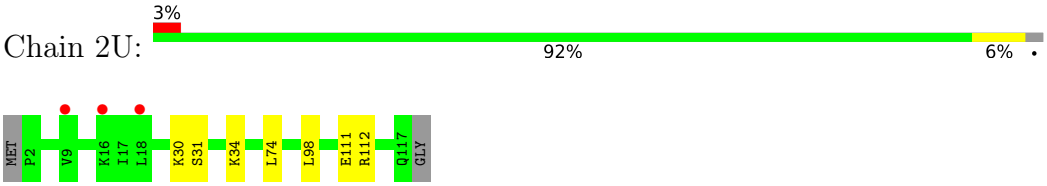
• Molecule 16: 50S ribosomal protein L20

Chain 1U:



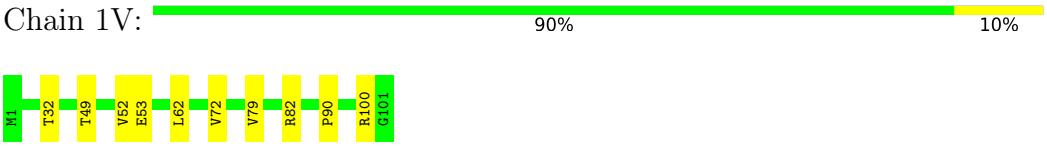
• Molecule 16: 50S ribosomal protein L20

Chain 2U:



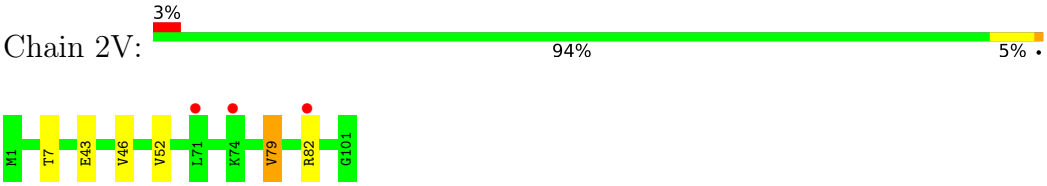
• Molecule 17: 50S ribosomal protein L21

Chain 1V:



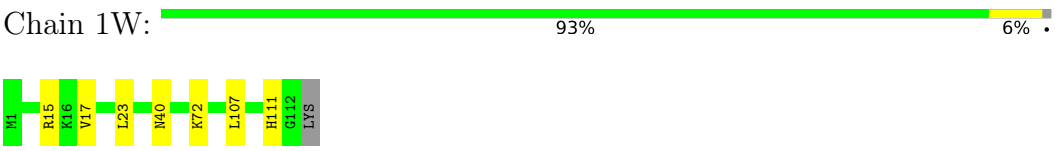
• Molecule 17: 50S ribosomal protein L21

Chain 2V:



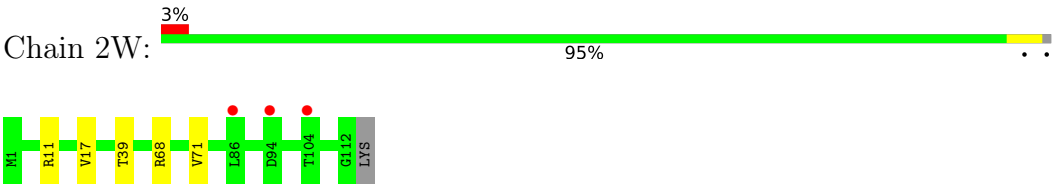
• Molecule 18: 50S ribosomal protein L22

Chain 1W:



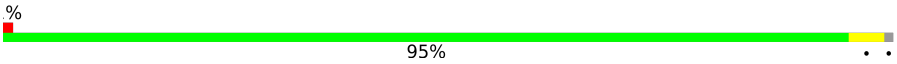
• Molecule 18: 50S ribosomal protein L22

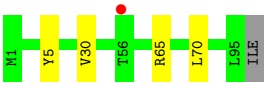
Chain 2W:



• Molecule 19: 50S ribosomal protein L23

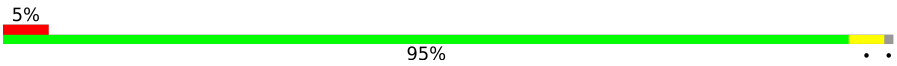
Chain 1X:

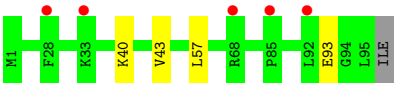




• Molecule 19: 50S ribosomal protein L23

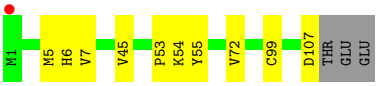
Chain 2X:





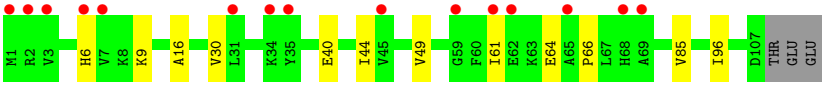
• Molecule 20: 50S ribosomal protein L24

Chain 1Y:



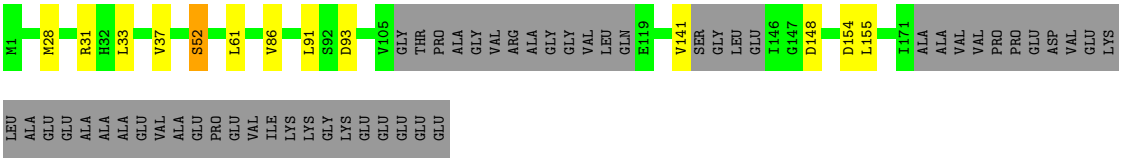
• Molecule 20: 50S ribosomal protein L24

Chain 2Y:



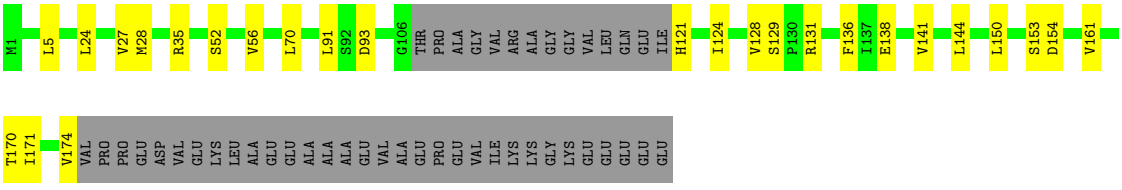
• Molecule 21: 50S ribosomal protein L25

Chain 1Z:



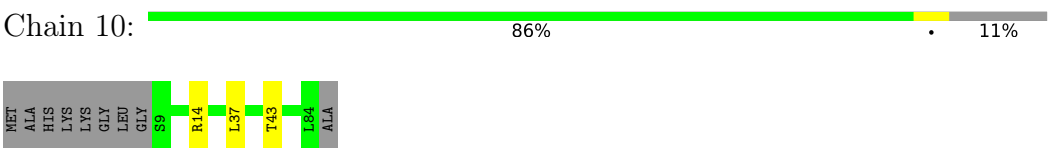
• Molecule 21: 50S ribosomal protein L25

Chain 2Z:



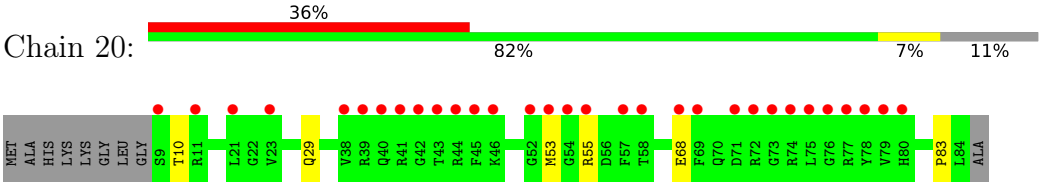
• Molecule 22: 50S ribosomal protein L27

Chain 10:



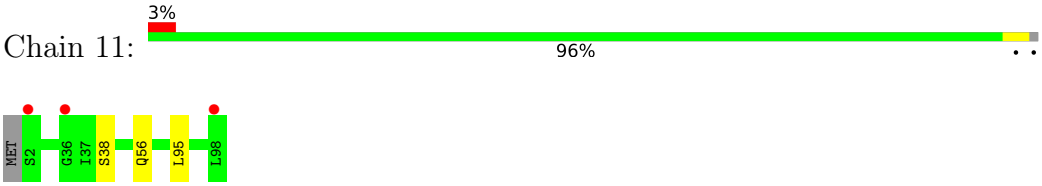
• Molecule 22: 50S ribosomal protein L27

Chain 20:



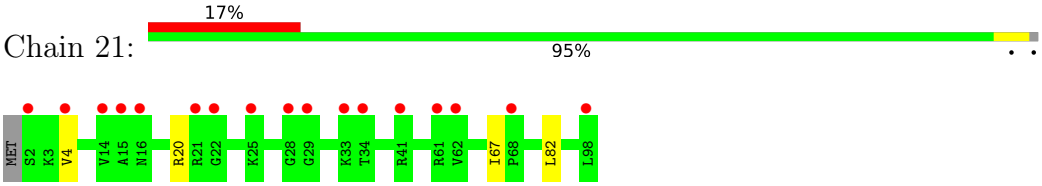
• Molecule 23: 50S ribosomal protein L28

Chain 11:



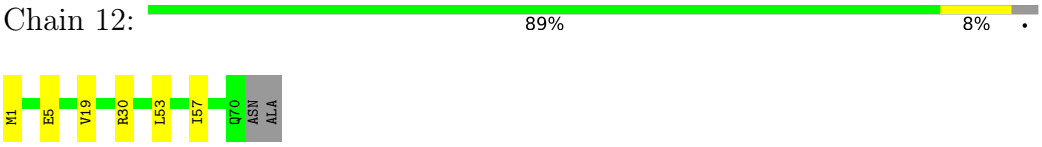
• Molecule 23: 50S ribosomal protein L28

Chain 21:



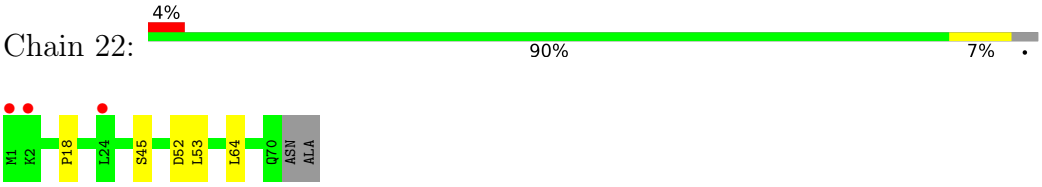
• Molecule 24: 50S ribosomal protein L29

Chain 12:



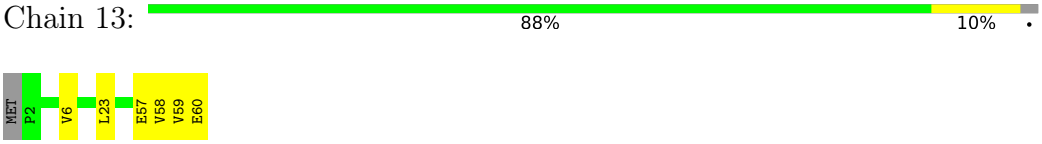
• Molecule 24: 50S ribosomal protein L29

Chain 22:



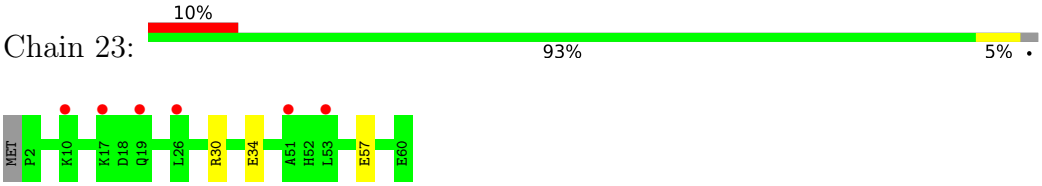
• Molecule 25: 50S ribosomal protein L30

Chain 13:



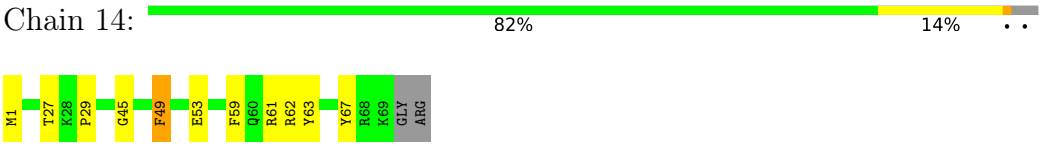
• Molecule 25: 50S ribosomal protein L30

Chain 23:



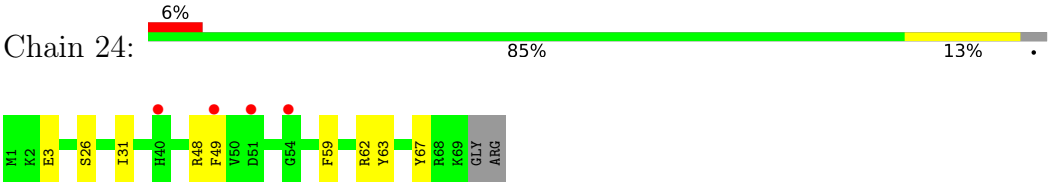
• Molecule 26: 50S ribosomal protein L31

Chain 14:



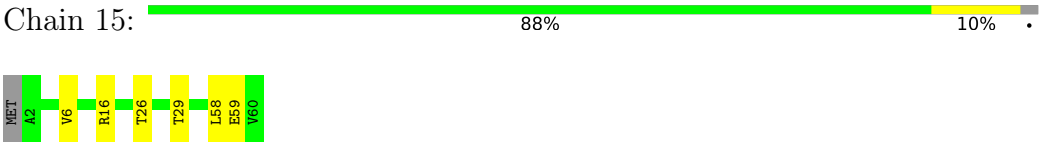
• Molecule 26: 50S ribosomal protein L31

Chain 24:



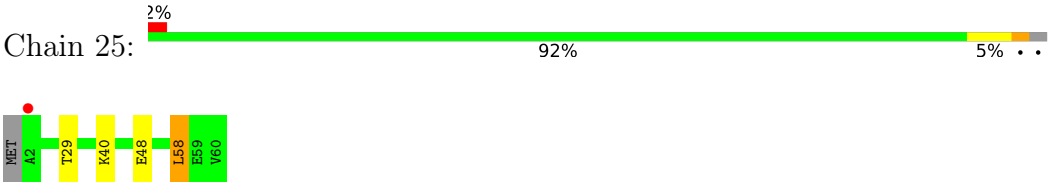
• Molecule 27: 50S ribosomal protein L32

Chain 15:



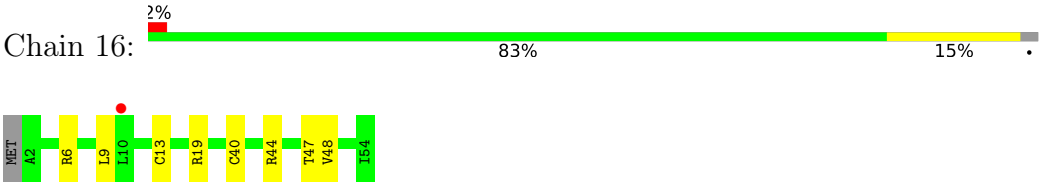
• Molecule 27: 50S ribosomal protein L32

Chain 25:



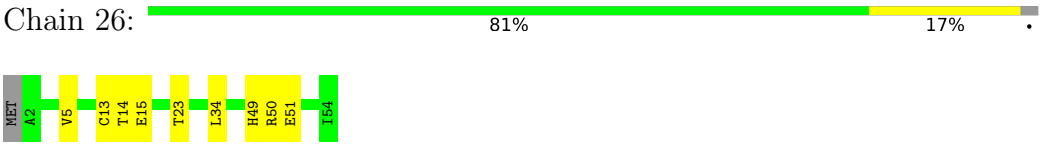
• Molecule 28: 50S ribosomal protein L33

Chain 16:



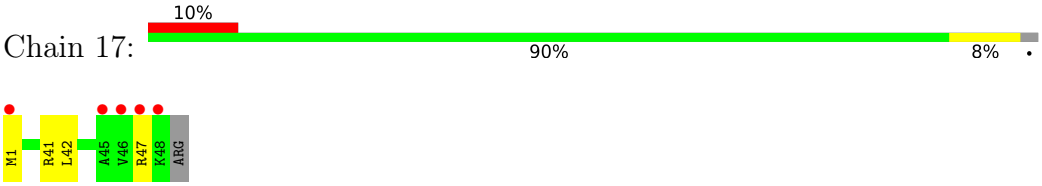
• Molecule 28: 50S ribosomal protein L33

Chain 26:



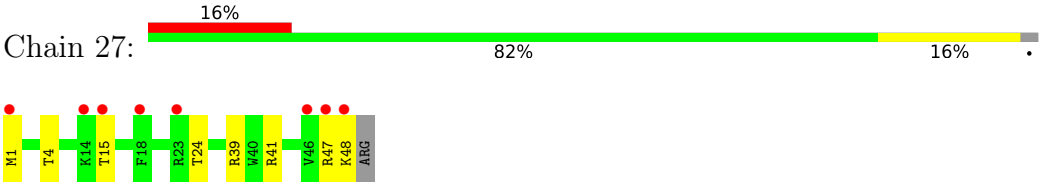
• Molecule 29: 50S ribosomal protein L34

Chain 17:



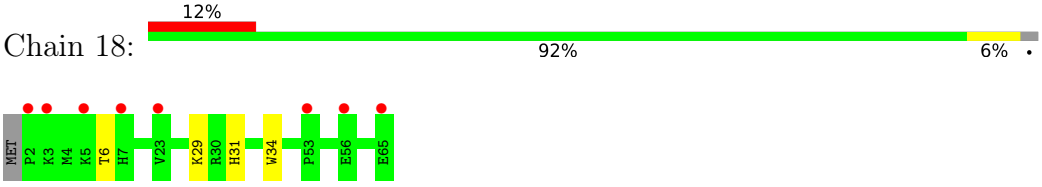
• Molecule 29: 50S ribosomal protein L34

Chain 27:



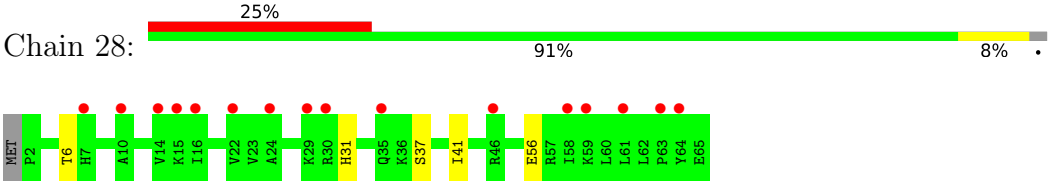
• Molecule 30: 50S ribosomal protein L35

Chain 18:



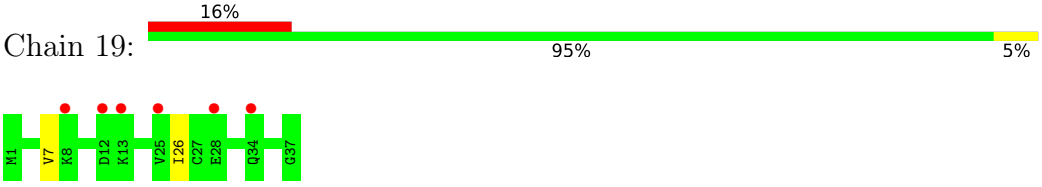
• Molecule 30: 50S ribosomal protein L35

Chain 28:



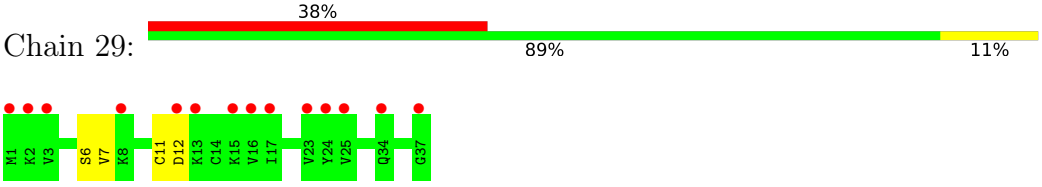
• Molecule 31: 50S ribosomal protein L36

Chain 19:



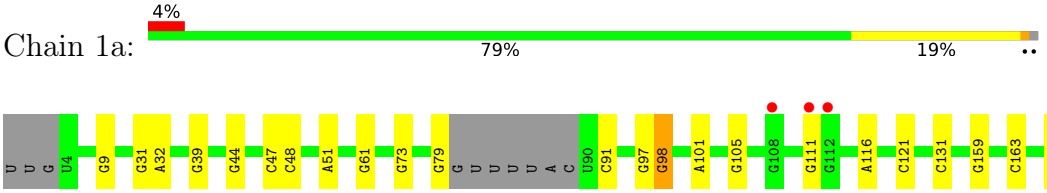
• Molecule 31: 50S ribosomal protein L36

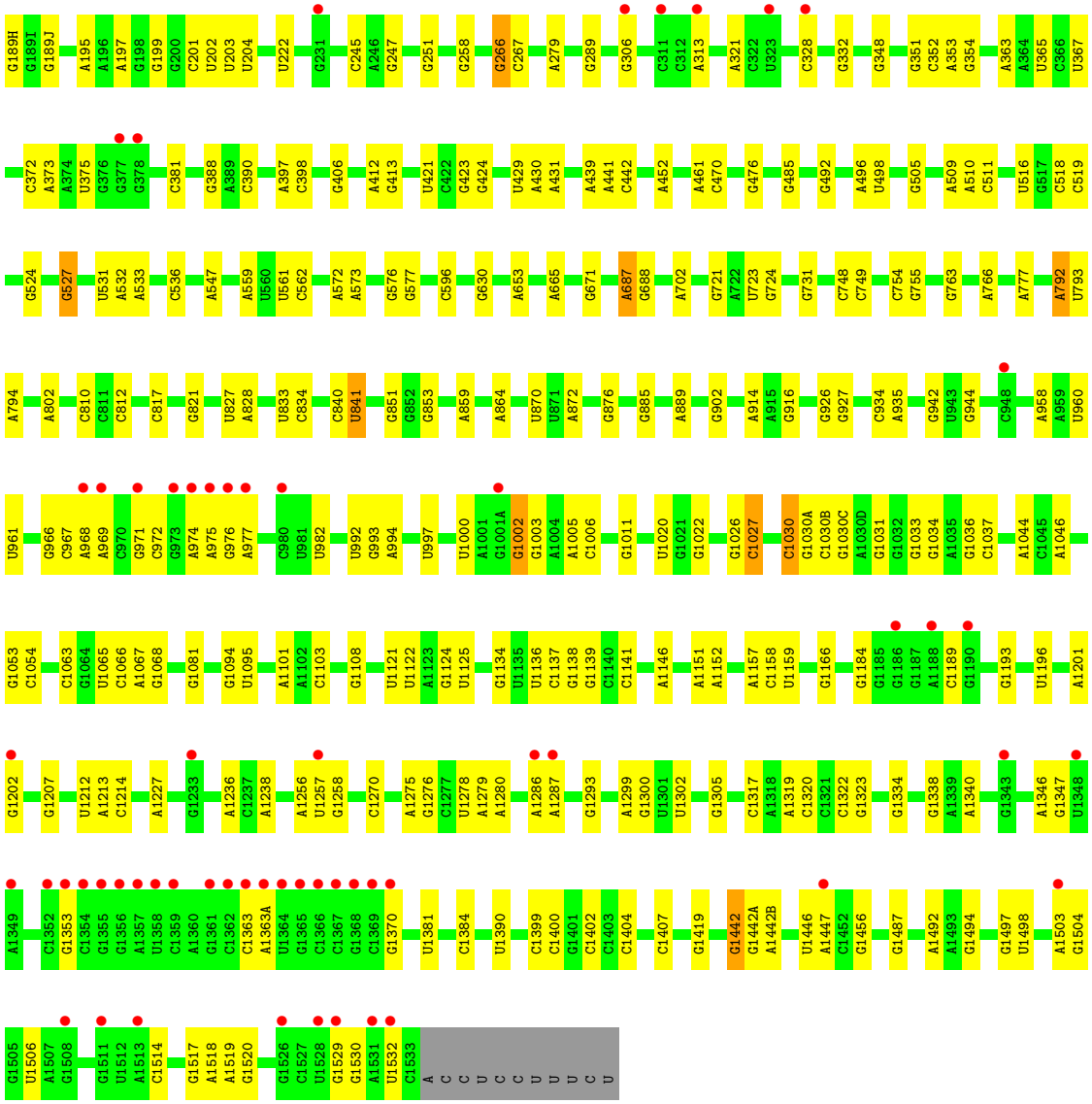
Chain 29:



• Molecule 32: 16S Ribosomal RNA

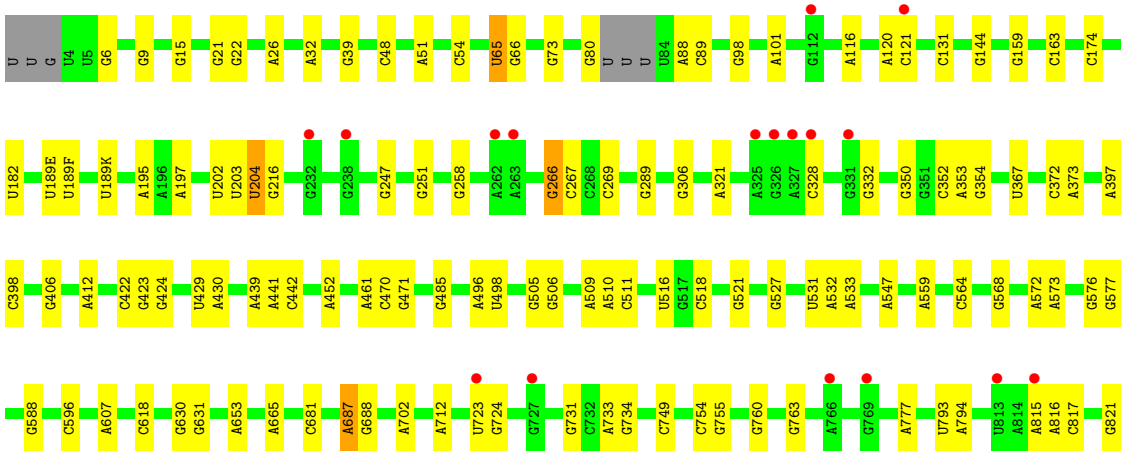
Chain 1a:

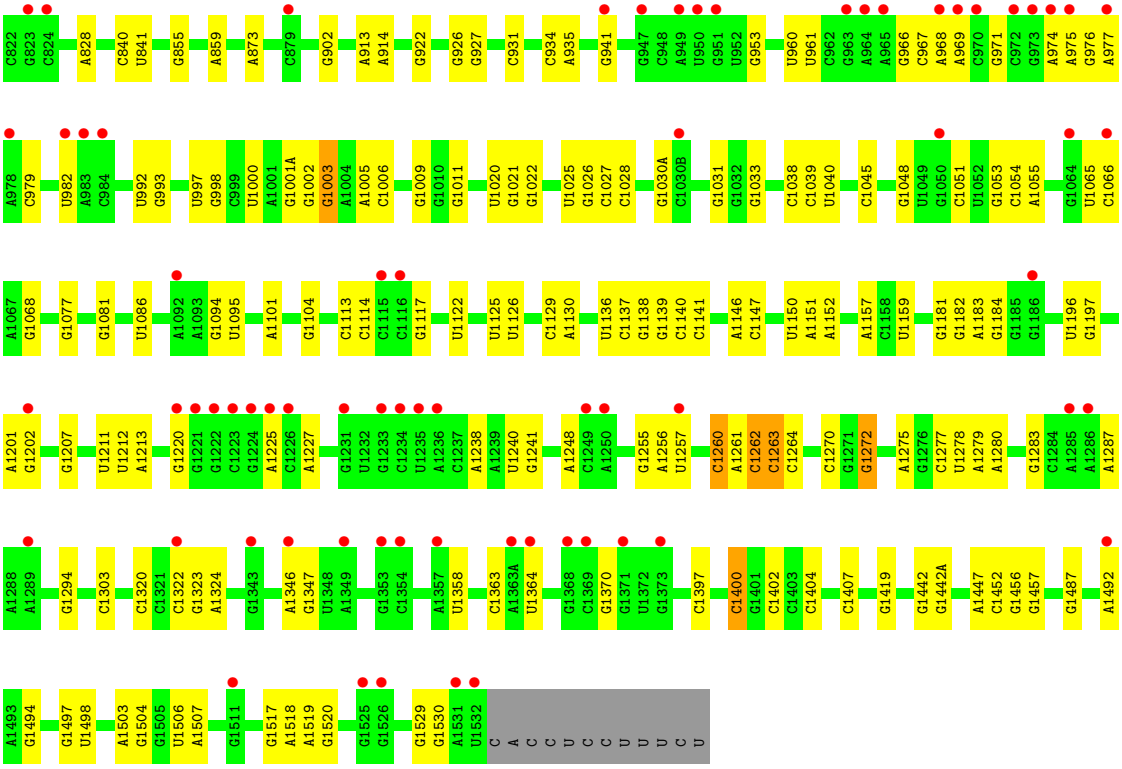




• Molecule 32: 16S Ribosomal RNA

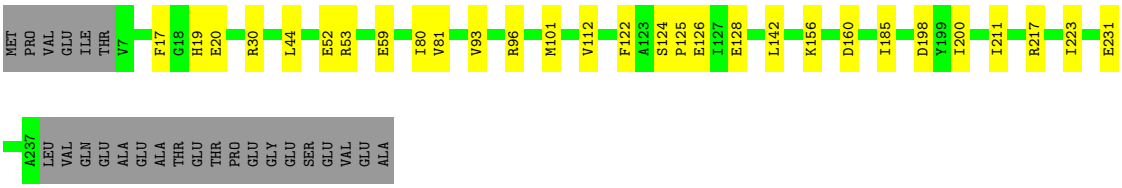
Chain 2a:





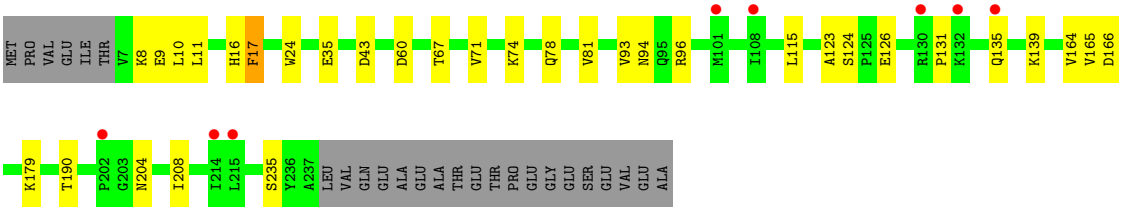
• Molecule 33: 30S ribosomal protein S2

Chain 1b:



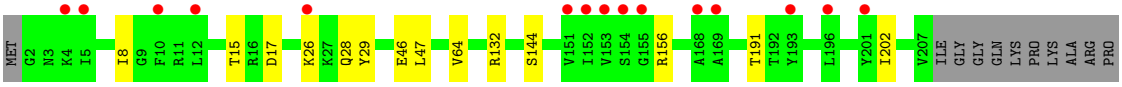
• Molecule 33: 30S ribosomal protein S2

Chain 2b:



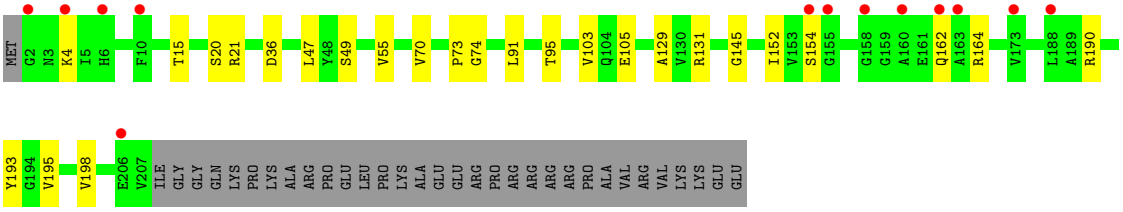
• Molecule 34: 30S ribosomal protein S3

Chain 1c:



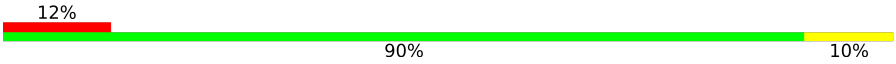
• Molecule 34: 30S ribosomal protein S3

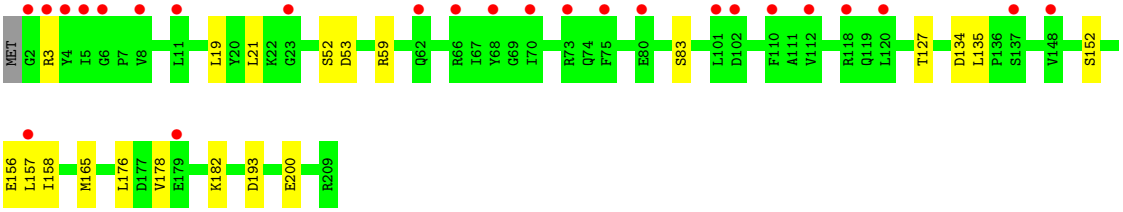
Chain 2c:



• Molecule 35: 30S ribosomal protein S4

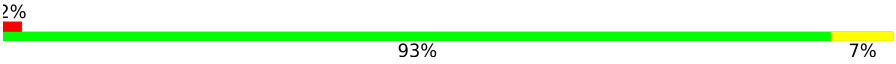
Chain 1d:

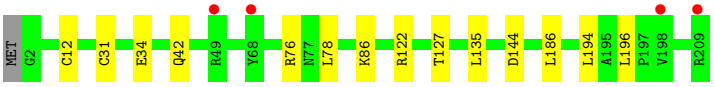




• Molecule 35: 30S ribosomal protein S4

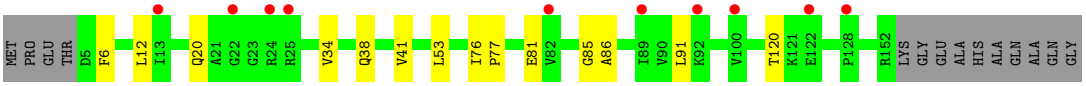
Chain 2d:





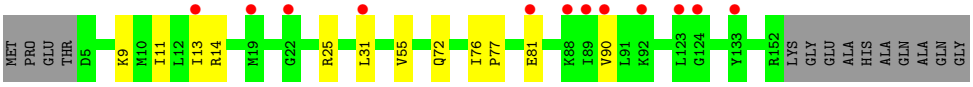
• Molecule 36: 30S ribosomal protein S5

Chain 1e:



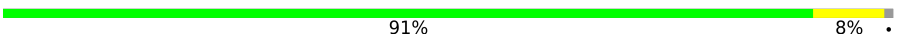
• Molecule 36: 30S ribosomal protein S5

Chain 2e:



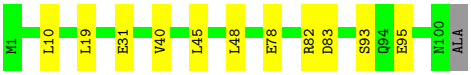
• Molecule 37: 30S ribosomal protein S6

Chain 1f:



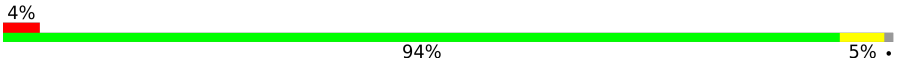
• Molecule 37: 30S ribosomal protein S6

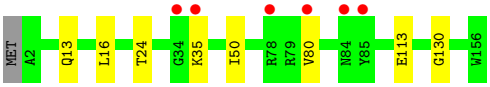
Chain 2f:



• Molecule 38: 30S ribosomal protein S7

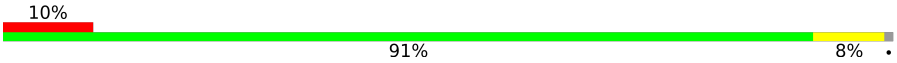
Chain 1g:

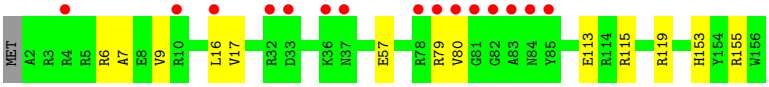




• Molecule 38: 30S ribosomal protein S7

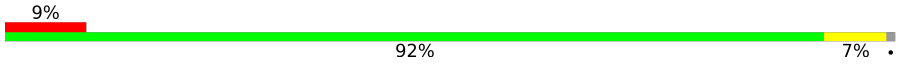
Chain 2g:

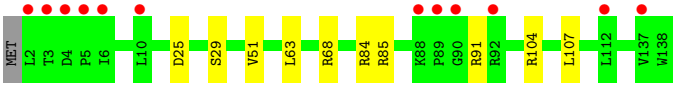




• Molecule 39: 30S ribosomal protein S8

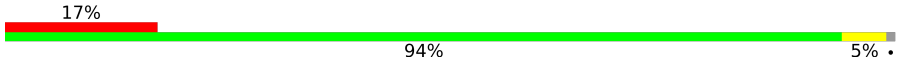
Chain 1h:

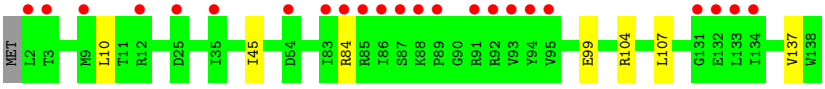




• Molecule 39: 30S ribosomal protein S8

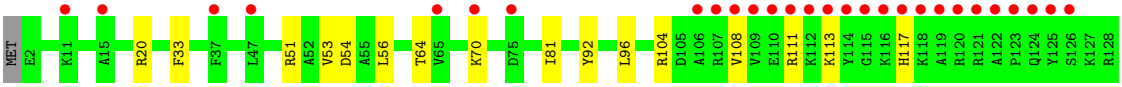
Chain 2h:





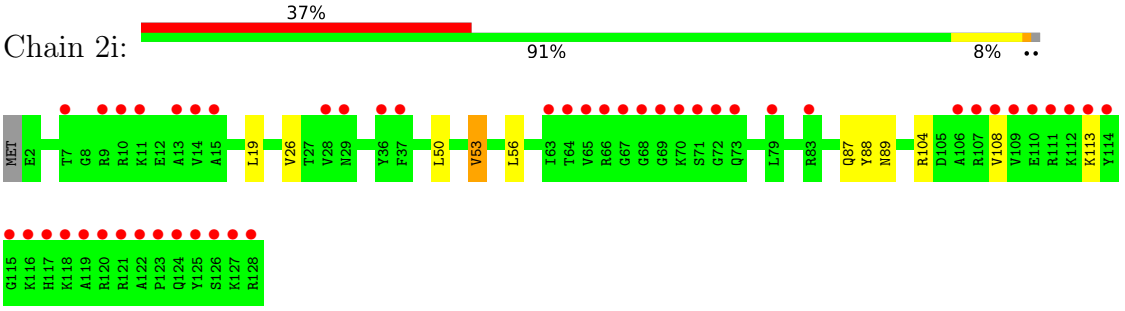
• Molecule 40: 30S ribosomal protein S9

Chain 1i:



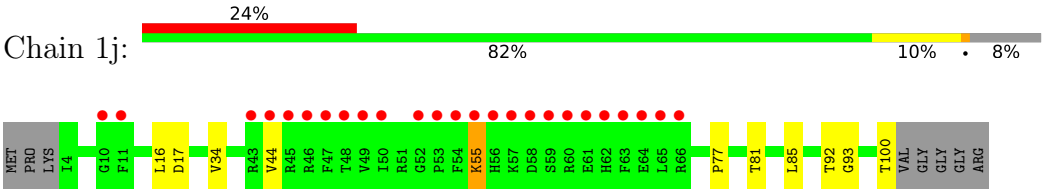
• Molecule 40: 30S ribosomal protein S9

Chain 2i:



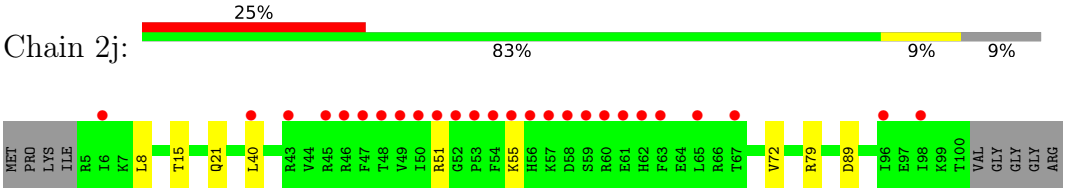
• Molecule 41: 30S ribosomal protein S10

Chain 1j:



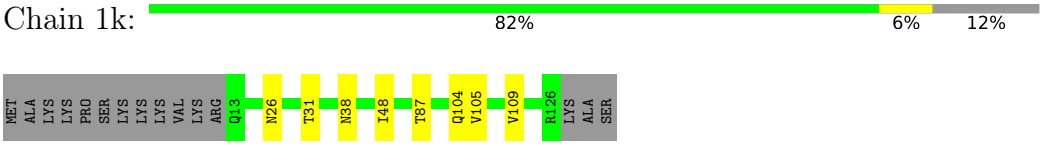
• Molecule 41: 30S ribosomal protein S10

Chain 2j:



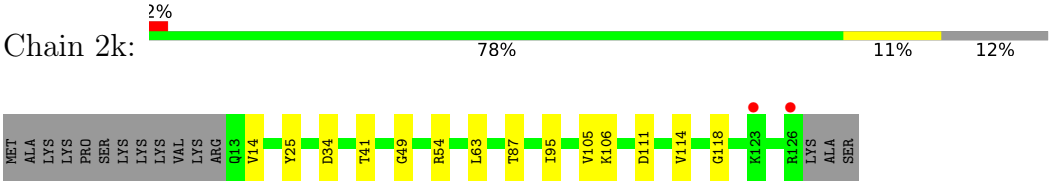
• Molecule 42: 30S ribosomal protein S11

Chain 1k:



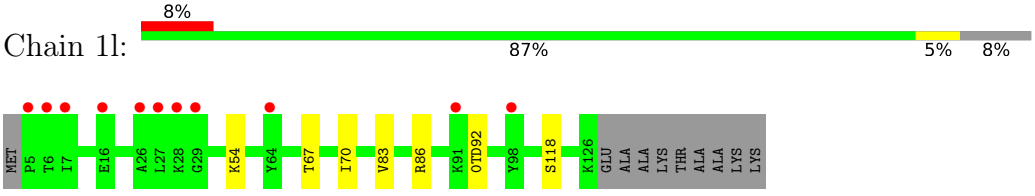
• Molecule 42: 30S ribosomal protein S11

Chain 2k:



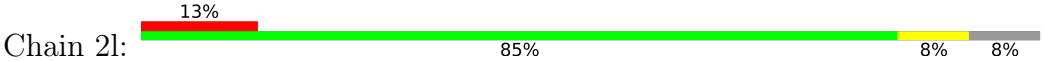
• Molecule 43: 30S ribosomal protein S12

Chain 1l:



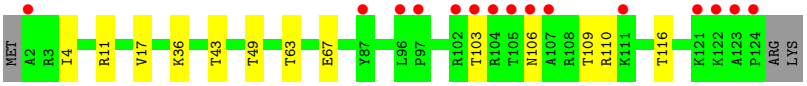
• Molecule 43: 30S ribosomal protein S12

Chain 2l:



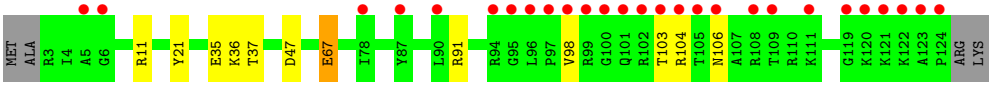
• Molecule 44: 30S ribosomal protein S13

Chain 1m:



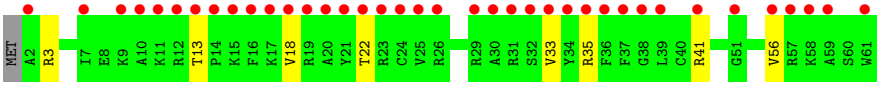
• Molecule 44: 30S ribosomal protein S13

Chain 2m:



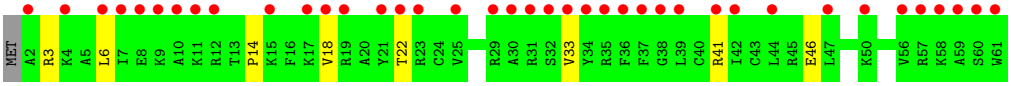
• Molecule 45: 30S ribosomal protein S14 type Z

Chain 1n:



• Molecule 45: 30S ribosomal protein S14 type Z

Chain 2n:

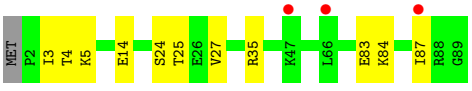


• Molecule 46: 30S ribosomal protein S15

Chain 1o:

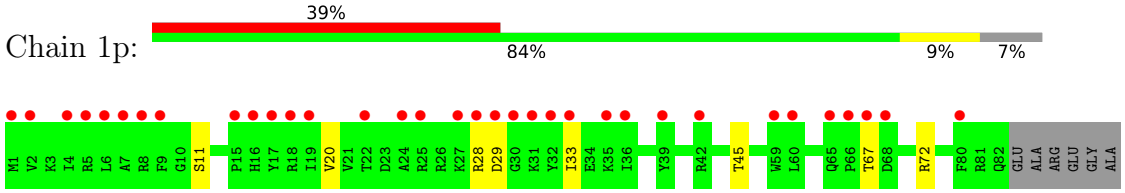
• Molecule 46: 30S ribosomal protein S15

Chain 2o:



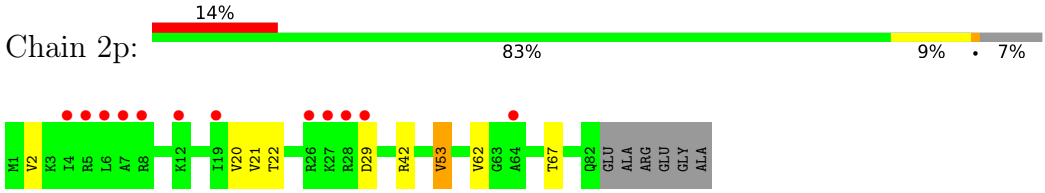
• Molecule 47: 30S ribosomal protein S16

Chain 1p:



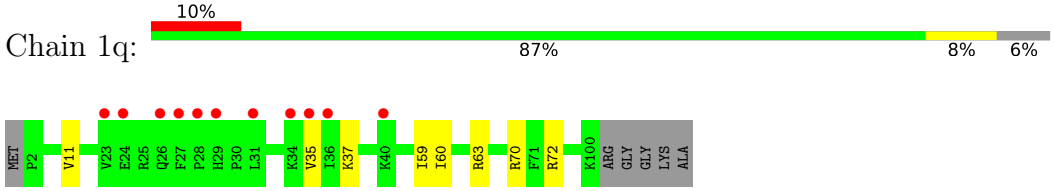
• Molecule 47: 30S ribosomal protein S16

Chain 2p:



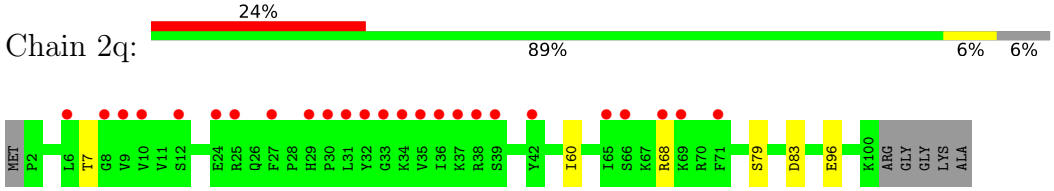
• Molecule 48: 30S ribosomal protein S17

Chain 1q:



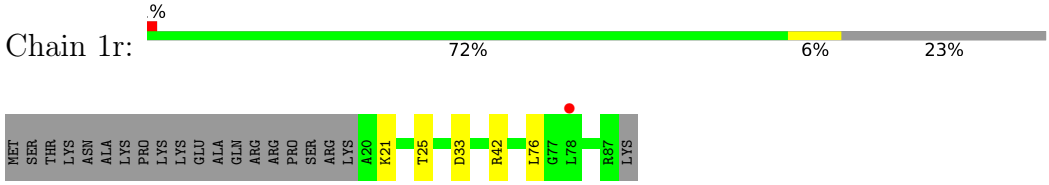
• Molecule 48: 30S ribosomal protein S17

Chain 2q:



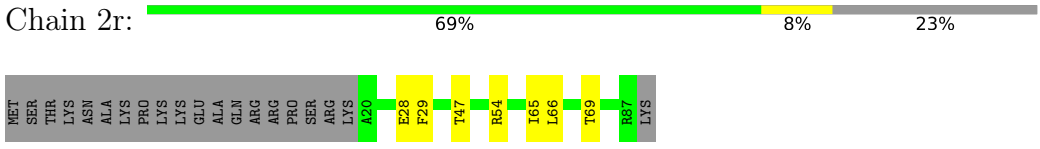
• Molecule 49: 30S ribosomal protein S18

Chain 1r:



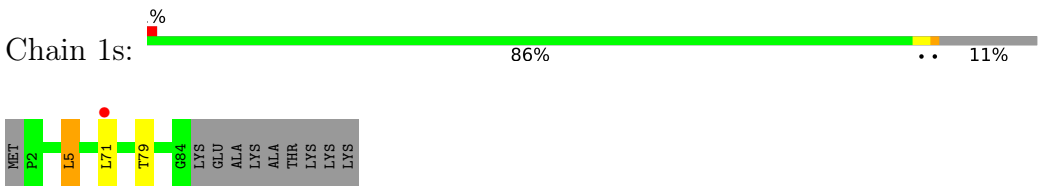
• Molecule 49: 30S ribosomal protein S18

Chain 2r:



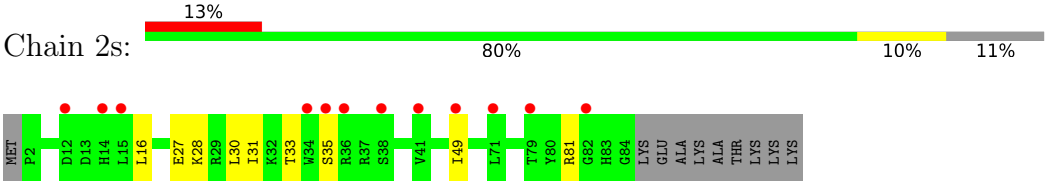
• Molecule 50: 30S ribosomal protein S19

Chain 1s:



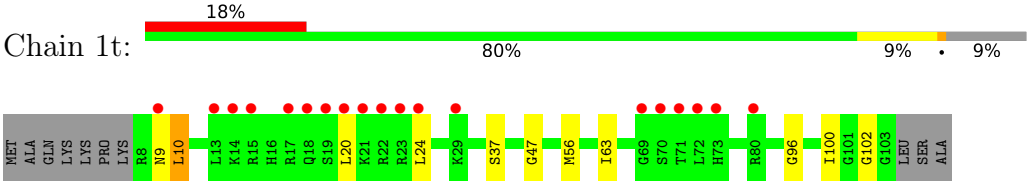
• Molecule 50: 30S ribosomal protein S19

Chain 2s:



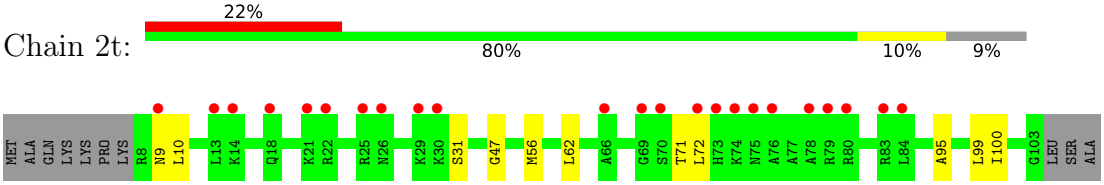
• Molecule 51: 30S ribosomal protein S20

Chain 1t:



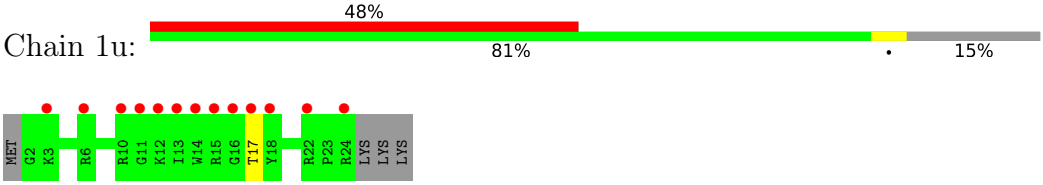
• Molecule 51: 30S ribosomal protein S20

Chain 2t:



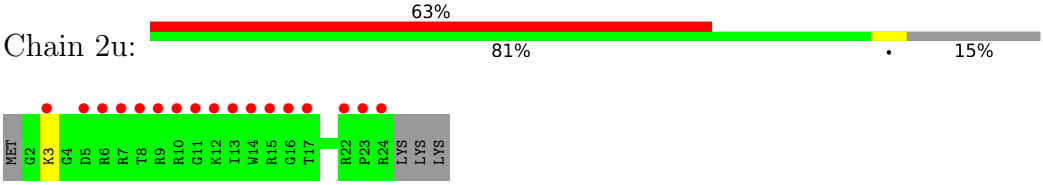
• Molecule 52: 30S ribosomal protein Thx

Chain 1u:



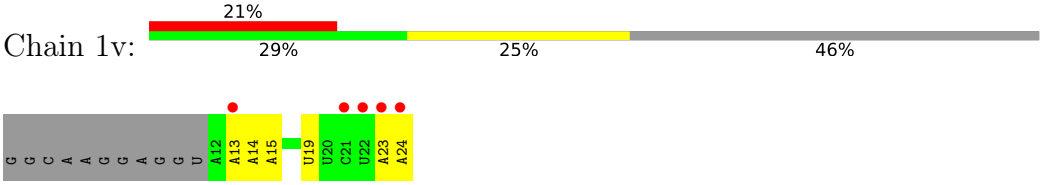
• Molecule 52: 30S ribosomal protein Thx

Chain 2u:



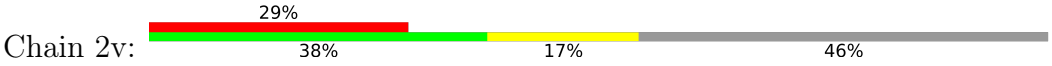
• Molecule 53: mRNA

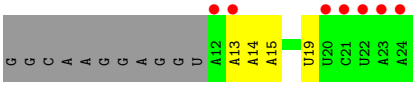
Chain 1v:



• Molecule 53: mRNA

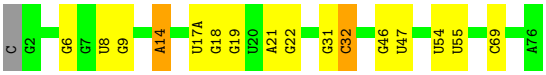
Chain 2v:





• Molecule 54: P-site tRNA

Chain 1x:

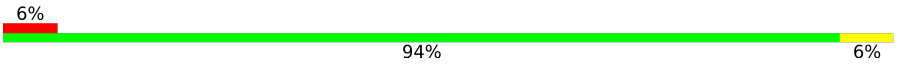


• Molecule 54: P-site tRNA

Chain 2x:

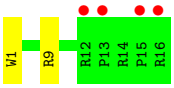
• Molecule 55: Bac7-001

Chain 1z:



• Molecule 55: Bac7-001

Chain 2z:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	209.09Å 449.88Å 621.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	76.76 – 3.00 255.62 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.4 (76.76-3.00) 99.4 (255.62-3.00)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.28 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.226 , 0.285 0.226 , 0.285	Depositor DCC
R_{free} test set	57578 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	68.0	Xtriage
Anisotropy	0.305	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 56.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.81	EDS
Total number of atoms	293228	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.47% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	1A	0.50	1/69009 (0.0%)	0.94	47/107712 (0.0%)
1	2A	0.41	0/67293	0.90	33/105034 (0.0%)
2	1B	0.45	1/2882 (0.0%)	0.90	0/4494
2	2B	0.44	1/2879 (0.0%)	0.94	2/4487 (0.0%)
3	1D	0.37	0/2186	0.55	0/2944
3	2D	0.32	0/2186	0.53	1/2944 (0.0%)
4	1E	0.34	0/1592	0.53	0/2149
4	2E	0.30	0/1592	0.51	0/2149
5	1F	0.34	0/1619	0.50	0/2193
5	2F	0.31	0/1615	0.50	0/2188
6	1G	0.31	0/1448	0.51	0/1957
6	2G	0.32	0/1453	0.51	0/1963
7	1H	0.33	0/1356	0.50	0/1834
7	2H	0.29	0/1356	0.47	0/1834
8	1I	0.30	0/1112	0.51	0/1514
8	2I	0.31	0/1079	0.47	0/1475
9	1N	0.34	0/1144	0.48	0/1543
9	2N	0.29	0/1144	0.49	0/1543
10	1O	0.35	0/943	0.54	0/1269
10	2O	0.33	0/943	0.56	0/1269
11	1P	0.34	0/1152	0.58	0/1533
11	2P	0.31	0/1152	0.54	0/1533
12	1Q	0.34	0/1143	0.52	0/1527
12	2Q	0.31	0/1143	0.53	0/1527
13	1R	0.30	0/982	0.51	0/1312
13	2R	0.29	0/982	0.49	0/1312
14	1S	0.30	0/883	0.49	0/1176
14	2S	0.32	0/880	0.51	0/1172
15	1T	0.32	0/1105	0.51	0/1477
15	2T	0.30	0/1097	0.47	0/1468
16	1U	0.34	0/977	0.49	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	2U	0.28	0/977	0.45	0/1301
17	1V	0.34	0/782	0.54	0/1049
17	2V	0.30	0/782	0.50	0/1049
18	1W	0.34	0/897	0.51	0/1205
18	2W	0.30	0/897	0.46	0/1205
19	1X	0.37	0/764	0.55	0/1025
19	2X	0.30	0/764	0.50	0/1025
20	1Y	0.32	0/819	0.51	0/1095
20	2Y	0.31	0/819	0.50	0/1095
21	1Z	0.32	0/1267	0.52	0/1717
21	2Z	0.33	0/1299	0.51	0/1763
22	10	0.35	0/612	0.53	0/816
22	20	0.33	0/612	0.50	0/816
23	11	0.34	0/762	0.51	0/1014
23	21	0.30	0/762	0.50	0/1014
24	12	0.31	0/590	0.49	0/781
24	22	0.32	0/590	0.43	0/781
25	13	0.31	0/474	0.51	0/635
25	23	0.29	0/469	0.47	0/630
26	14	0.35	0/565	0.57	0/761
26	24	0.34	0/545	0.55	0/737
27	15	0.33	0/469	0.52	0/635
27	25	0.34	0/469	0.55	1/635 (0.2%)
28	16	0.35	0/460	0.54	0/613
28	26	0.30	0/456	0.49	0/608
29	17	0.33	0/426	0.52	0/561
29	27	0.28	0/426	0.49	0/561
30	18	0.35	0/525	0.52	0/691
30	28	0.30	0/525	0.48	0/691
31	19	0.33	0/310	0.52	0/407
31	29	0.31	0/310	0.54	0/407
32	1a	0.39	0/35795	0.91	41/55864 (0.1%)
32	2a	0.38	2/35886 (0.0%)	0.93	46/56005 (0.1%)
33	1b	0.30	0/1881	0.51	0/2542
33	2b	0.30	0/1860	0.49	0/2518
34	1c	0.30	0/1572	0.48	0/2126
34	2c	0.30	0/1566	0.51	0/2119
35	1d	0.30	0/1685	0.48	0/2262
35	2d	0.29	0/1704	0.48	0/2284
36	1e	0.29	0/1145	0.52	0/1543
36	2e	0.32	0/1149	0.51	0/1548
37	1f	0.30	0/823	0.50	0/1115
37	2f	0.30	0/829	0.47	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	1g	0.29	0/1250	0.45	0/1679
38	2g	0.29	0/1254	0.44	0/1683
39	1h	0.29	0/1108	0.50	0/1494
39	2h	0.28	0/1108	0.47	0/1494
40	1i	0.32	0/1002	0.51	0/1346
40	2i	0.31	0/997	0.51	0/1343
41	1j	0.30	0/722	0.52	0/982
41	2j	0.31	0/727	0.49	0/988
42	1k	0.30	0/844	0.49	0/1145
42	2k	0.31	0/848	0.49	0/1149
43	1l	0.32	0/937	0.50	0/1260
43	2l	0.30	0/937	0.51	0/1260
44	1m	0.29	0/969	0.49	0/1302
44	2m	0.30	0/961	0.48	0/1291
45	1n	0.32	0/501	0.48	0/664
45	2n	0.28	0/501	0.51	0/664
46	1o	0.27	0/739	0.44	0/985
46	2o	0.28	0/739	0.45	0/985
47	1p	0.29	0/697	0.49	0/939
47	2p	0.29	0/693	0.48	0/935
48	1q	0.32	0/836	0.52	0/1117
48	2q	0.30	0/836	0.46	0/1117
49	1r	0.30	0/560	0.50	0/746
49	2r	0.30	0/560	0.46	0/746
50	1s	0.28	0/667	0.56	1/900 (0.1%)
50	2s	0.31	0/661	0.55	0/893
51	1t	0.29	0/730	0.43	0/965
51	2t	0.28	0/729	0.47	0/965
52	1u	0.28	0/203	0.50	0/266
52	2u	0.29	0/203	0.46	0/266
53	1v	0.48	0/310	0.95	0/480
53	2v	0.61	0/310	0.94	0/480
54	1x	0.49	0/1725	1.06	10/2689 (0.4%)
54	2x	0.51	1/1725 (0.1%)	1.15	18/2689 (0.7%)
55	1z	0.33	0/150	0.49	0/205
55	2z	0.28	0/150	0.50	0/205
All	All	0.40	6/310535 (0.0%)	0.83	200/464522 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
33	1b	0	1
51	2t	0	1
All	All	0	2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2B	1	U	OP3-P	-10.23	1.48	1.61
2	1B	1	U	OP3-P	-10.15	1.49	1.61
32	2a	1272	G	N1-C2	-6.68	1.32	1.37
32	2a	1272	G	C6-N1	-5.89	1.35	1.39
54	2x	22	G	N7-C5	5.51	1.42	1.39
1	1A	2790	A	N9-C4	5.20	1.41	1.37

All (200) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	1263	C	N1-C2-O2	18.39	129.94	118.90
32	2a	1272	G	N3-C2-N2	15.64	130.85	119.90
32	2a	1272	G	C5-C6-O6	14.71	137.43	128.60
32	2a	1272	G	N1-C2-N2	-13.13	104.38	116.20
2	2B	80	U	O4'-C1'-N1	12.02	117.81	108.20
32	2a	1263	C	C2-N3-C4	11.02	125.41	119.90
32	2a	1263	C	N3-C2-O2	-10.39	114.63	121.90
32	2a	1272	G	C6-N1-C2	9.26	130.66	125.10
32	1a	1030(B)	C	N1-C2-O2	8.73	124.14	118.90
32	1a	1027	C	N3-C4-C5	-8.65	118.44	121.90
32	2a	1272	G	C5-C6-N1	-8.64	107.18	111.50
1	1A	1075	C	N1-C2-O2	8.56	124.03	118.90
54	2x	46	G	C6-N1-C2	-8.53	119.98	125.10
32	1a	1030(B)	C	C2-N1-C1'	8.50	128.15	118.80
54	2x	14	A	C4-C5-C6	8.39	121.20	117.00
1	1A	2167	U	C2-N1-C1'	7.99	127.29	117.70
32	2a	1272	G	C4-N9-C1'	7.89	136.75	126.50
54	2x	22	G	N1-C6-O6	-7.79	115.22	119.90
1	2A	2136	C	N1-C2-O2	7.72	123.53	118.90
1	1A	1063	G	C5-C6-O6	7.66	133.20	128.60
32	1a	1027	C	N3-C2-O2	-7.61	116.57	121.90
32	2a	1272	G	N1-C6-O6	-7.52	115.39	119.90
32	2a	1263	C	C5-C6-N1	7.48	124.74	121.00
32	1a	1030(B)	C	C6-N1-C2	-7.47	117.31	120.30
32	1a	266	G	P-O3'-C3'	7.46	128.65	119.70
32	1a	1030(B)	C	N3-C2-O2	-7.43	116.70	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2A	2473	U	C2-N1-C1'	7.29	126.44	117.70
1	1A	512	G	O4'-C1'-N9	7.24	113.99	108.20
32	2a	1272	G	C8-N9-C1'	-7.14	117.72	127.00
32	2a	754	C	C2-N1-C1'	6.89	126.38	118.80
1	1A	847	U	C2-N1-C1'	6.89	125.97	117.70
54	1x	46	G	C6-N1-C2	-6.83	121.00	125.10
1	1A	1063	G	C6-N1-C2	6.82	129.19	125.10
54	1x	14	A	C5-N7-C8	6.73	107.27	103.90
1	1A	2167	U	N3-C2-O2	-6.72	117.50	122.20
1	2A	2473	U	N3-C2-O2	-6.69	117.51	122.20
1	1A	2167	U	N1-C2-O2	6.66	127.46	122.80
1	2A	2155	G	N3-C2-N2	6.64	124.55	119.90
32	2a	1263	C	C5-C4-N4	6.61	124.83	120.20
54	2x	14	A	C5-N7-C8	6.60	107.20	103.90
54	2x	22	G	C4-C5-C6	-6.59	114.85	118.80
1	2A	2149	G	N3-C4-N9	6.54	129.92	126.00
54	2x	22	G	C8-N9-C1'	6.52	135.48	127.00
54	2x	14	A	N1-C6-N6	6.51	122.51	118.60
32	2a	1263	C	C2-N1-C1'	6.51	125.96	118.80
27	25	58	LEU	CA-CB-CG	6.50	130.24	115.30
1	1A	1075	C	C2-N3-C4	6.46	123.13	119.90
32	1a	1027	C	C5-C4-N4	6.46	124.72	120.20
1	1A	1176	G	OP1-P-O3'	6.44	119.36	105.20
1	2A	2473	U	N1-C2-O2	6.40	127.28	122.80
32	2a	1225	A	N1-C6-N6	-6.34	114.80	118.60
54	1x	22	G	C8-N9-C1'	6.33	135.22	127.00
1	1A	121	G	C4-N9-C1'	6.30	134.69	126.50
54	2x	46	G	N9-C4-C5	6.22	107.89	105.40
1	2A	2136	C	N3-C2-O2	-6.20	117.56	121.90
32	1a	1034	G	N9-C4-C5	-6.19	102.92	105.40
54	1x	22	G	N3-C4-N9	-6.18	122.29	126.00
32	1a	841	U	C5-C6-N1	6.17	125.78	122.70
1	1A	1905	C	C2-N1-C1'	6.17	125.58	118.80
54	2x	46	G	N3-C2-N2	-6.16	115.59	119.90
54	1x	22	G	N1-C6-O6	-6.15	116.21	119.90
1	2A	2155	G	C6-N1-C2	6.12	128.77	125.10
32	2a	1225	A	C5-C6-N6	6.02	128.51	123.70
54	1x	22	G	C6-C5-N7	6.00	134.00	130.40
32	2a	204	U	C2-N1-C1'	5.98	124.87	117.70
1	1A	2689	U	P-O3'-C3'	5.95	126.83	119.70
1	2A	2168	G	C4-N9-C1'	5.94	134.22	126.50
32	2a	1028	C	C2-N3-C4	5.94	122.87	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	1176	G	P-O3'-C3'	5.88	126.75	119.70
32	2a	1260	C	C6-N1-C2	-5.87	117.95	120.30
1	2A	2206	G	C4-N9-C1'	-5.86	118.88	126.50
32	2a	266	G	P-O3'-C3'	5.86	126.73	119.70
32	1a	1034	G	N3-C2-N2	5.85	124.00	119.90
1	1A	1905	C	N1-C2-O2	5.85	122.41	118.90
32	2a	1263	C	N3-C4-N4	-5.85	113.90	118.00
1	1A	1075	C	N3-C2-O2	-5.85	117.81	121.90
32	1a	1036	G	N1-C6-O6	-5.85	116.39	119.90
1	2A	2149	G	C4-N9-C1'	5.84	134.10	126.50
1	2A	2149	G	C6-C5-N7	-5.84	126.90	130.40
54	2x	22	G	C6-C5-N7	5.84	133.90	130.40
32	1a	754	C	C2-N1-C1'	5.83	125.22	118.80
32	2a	979	C	C6-N1-C2	-5.82	117.97	120.30
1	1A	1064	C	N1-C2-O2	5.81	122.38	118.90
54	2x	46	G	C4-C5-N7	-5.81	108.48	110.80
1	2A	2155	G	N3-C4-N9	5.80	129.48	126.00
1	1A	1063	G	N3-C2-N2	5.78	123.94	119.90
1	1A	1249	U	O5'-P-OP1	-5.77	100.50	105.70
32	2a	1264	C	N1-C2-O2	5.77	122.36	118.90
1	2A	1372	U	C5-C4-O4	-5.76	122.44	125.90
1	2A	1313	U	C2-N1-C1'	5.76	124.61	117.70
54	2x	14	A	C5-C6-N1	-5.75	114.83	117.70
1	1A	889	C	N1-C2-O2	5.75	122.35	118.90
32	1a	1030	C	C5-C4-N4	5.74	124.22	120.20
32	2a	1126	U	C2-N1-C1'	5.73	124.58	117.70
1	2A	1530	C	P-O3'-C3'	5.72	126.56	119.70
54	2x	22	G	C4-N9-C1'	-5.71	119.07	126.50
1	1A	784	A	P-O3'-C3'	5.71	126.55	119.70
32	1a	1030	C	C2-N3-C4	5.70	122.75	119.90
1	1A	2848	G	O4'-C1'-N9	5.70	112.76	108.20
32	1a	1067	A	P-O3'-C3'	5.68	126.52	119.70
54	1x	22	G	C4-C5-C6	-5.67	115.40	118.80
1	2A	512	G	O4'-C1'-N9	5.65	112.72	108.20
32	1a	1034	G	C6-N1-C2	5.63	128.48	125.10
1	2A	1022	G	N3-C4-N9	-5.62	122.63	126.00
32	1a	1011	G	N3-C4-N9	5.59	129.36	126.00
32	1a	1158	C	C2-N1-C1'	5.59	124.95	118.80
1	1A	1105	U	C5-C4-O4	-5.58	122.55	125.90
32	2a	1028	C	C5-C4-N4	5.55	124.09	120.20
1	1A	897	C	N1-C2-O2	-5.55	115.57	118.90
32	2a	1263	C	C6-N1-C2	-5.55	118.08	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	1131	G	O4'-C1'-N9	5.54	112.64	108.20
32	2a	65	U	P-O3'-C3'	5.53	126.33	119.70
1	1A	548	A	P-O3'-C3'	5.52	126.33	119.70
32	1a	1011	G	N3-C4-C5	-5.52	125.84	128.60
1	1A	2790	A	C2-N3-C4	5.51	113.35	110.60
32	1a	1034	G	N3-C4-N9	5.48	129.29	126.00
1	1A	2134	A	P-O3'-C3'	5.48	126.28	119.70
1	1A	34	C	N1-C2-O2	5.47	122.18	118.90
32	2a	1033	G	C6-N1-C2	5.46	128.37	125.10
1	2A	2321	G	C4-N9-C1'	5.45	133.58	126.50
1	1A	2175	C	N1-C2-O2	5.44	122.17	118.90
32	2a	1263	C	N1-C2-N3	-5.44	115.39	119.20
1	1A	2035	G	O4'-C1'-N9	5.43	112.55	108.20
32	2a	1201	A	P-O3'-C3'	5.42	126.21	119.70
1	1A	1992	G	P-O3'-C3'	5.42	126.21	119.70
1	1A	1653	G	P-O3'-C3'	5.40	126.18	119.70
32	2a	754	C	N1-C2-O2	5.40	122.14	118.90
54	1x	22	G	C4-N9-C1'	-5.39	119.49	126.50
1	2A	945	A	O4'-C1'-N9	5.39	112.51	108.20
1	1A	2319	G	O4'-C1'-N9	5.38	112.51	108.20
54	2x	22	G	N3-C4-N9	-5.38	122.77	126.00
54	1x	14	A	C4-C5-C6	5.38	119.69	117.00
1	1A	1979	C	C6-N1-C2	-5.36	118.16	120.30
32	1a	841	U	C6-N1-C2	-5.36	117.78	121.00
32	1a	1027	C	C4-C5-C6	5.36	120.08	117.40
32	2a	913	A	P-O3'-C3'	5.35	126.12	119.70
1	2A	2128	C	C2-N3-C4	5.34	122.57	119.90
32	1a	1002	G	N3-C4-N9	5.33	129.20	126.00
1	2A	2149	G	C8-N9-C1'	-5.33	120.07	127.00
1	1A	121	G	C8-N9-C1'	-5.33	120.07	127.00
1	1A	2689	U	C6-N1-C2	-5.32	117.81	121.00
32	2a	1150	U	C5-C4-O4	5.31	129.08	125.90
32	2a	1262	C	N1-C2-O2	5.31	122.08	118.90
32	2a	266	G	N3-C4-C5	-5.30	125.95	128.60
32	1a	266	G	OP2-P-O3'	5.30	116.86	105.20
32	1a	365	U	C2-N1-C1'	5.30	124.06	117.70
32	1a	1034	G	C8-N9-C1'	-5.29	120.12	127.00
1	1A	1174	A	OP1-P-O3'	5.29	116.83	105.20
1	2A	90	U	N3-C2-O2	-5.28	118.51	122.20
32	2a	1262	C	C2-N1-C1'	5.27	124.60	118.80
32	2a	1003	G	C4-N9-C1'	5.26	133.33	126.50
32	1a	1030(B)	C	C6-N1-C1'	-5.25	114.50	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	1054	A	C6-N1-C2	-5.25	115.45	118.60
32	2a	687	A	P-O3'-C3'	5.24	125.99	119.70
1	1A	12	U	C2-N1-C1'	5.23	123.97	117.70
1	2A	228	A	P-O3'-C3'	5.23	125.97	119.70
32	1a	1034	G	C4-N9-C1'	5.21	133.28	126.50
1	2A	528	A	OP1-P-O3'	5.21	116.66	105.20
54	2x	22	G	C5-C6-N1	5.21	114.11	111.50
1	1A	226	G	O4'-C1'-N9	5.21	112.36	108.20
2	2B	71	C	N1-C2-O2	5.20	122.02	118.90
50	1s	5	LEU	CA-CB-CG	5.19	127.24	115.30
32	1a	1027	C	C6-N1-C2	-5.19	118.22	120.30
1	1A	2714	G	O5'-P-OP2	-5.18	101.04	105.70
1	1A	1074	G	C4-C5-N7	5.17	112.87	110.80
1	1A	847	U	N3-C2-O2	-5.15	118.59	122.20
32	1a	1030(B)	C	C5-C6-N1	5.15	123.58	121.00
32	2a	754	C	C6-N1-C1'	-5.15	114.62	120.80
32	1a	687	A	P-O3'-C3'	5.13	125.86	119.70
1	2A	1979	C	C6-N1-C2	-5.13	118.25	120.30
32	1a	1065	U	P-O3'-C3'	5.13	125.85	119.70
32	1a	748	C	P-O3'-C3'	5.12	125.85	119.70
54	2x	22	G	O4'-C1'-N9	5.12	112.30	108.20
32	1a	792	A	O4'-C1'-N9	5.12	112.30	108.20
32	1a	1442	G	P-O3'-C3'	5.12	125.84	119.70
32	2a	1225	A	C8-N9-C4	-5.11	103.75	105.80
32	1a	1036	G	C5-C6-O6	5.10	131.66	128.60
1	2A	1192	G	C8-N9-C4	5.10	108.44	106.40
32	1a	1514	C	C6-N1-C2	-5.10	118.26	120.30
1	2A	2155	G	N9-C4-C5	-5.10	103.36	105.40
32	1a	1011	G	C4-N9-C1'	5.08	133.10	126.50
1	1A	2101	G	C5-C6-O6	5.07	131.64	128.60
1	2A	2315	G	N3-C4-N9	5.07	129.04	126.00
1	1A	2149	G	N3-C4-N9	5.07	129.04	126.00
1	1A	1116	C	C5-C4-N4	-5.06	116.66	120.20
32	2a	1260	C	N1-C2-O2	5.06	121.94	118.90
32	2a	1260	C	C2-N1-C1'	5.06	124.36	118.80
3	2D	147	LEU	C-N-CA	5.06	134.34	121.70
1	2A	90	U	N1-C2-O2	5.05	126.34	122.80
1	2A	783	A	C2-N3-C4	5.05	113.13	110.60
54	2x	17	C	C2-N1-C1'	5.04	124.35	118.80
32	1a	98	G	N3-C4-N9	5.04	129.02	126.00
54	1x	14	A	C5-C6-N1	-5.03	115.18	117.70
1	2A	383	U	O4'-C1'-N1	5.03	112.22	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	1a	1027	C	N1-C2-O2	5.02	121.91	118.90
1	2A	2128	C	N1-C2-O2	5.01	121.91	118.90
54	2x	22	G	C5-N7-C8	-5.01	101.80	104.30
32	2a	979	C	C2-N1-C1'	5.01	124.31	118.80
32	2a	1260	C	C5-C6-N1	5.00	123.50	121.00
32	2a	1272	G	N3-C4-N9	5.00	129.00	126.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
33	1b	122	PHE	Peptide
51	2t	9	ASN	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%)	251 (92%)	21 (8%)	1 (0%)	34 72
3	2D	273/276 (99%)	245 (90%)	27 (10%)	1 (0%)	34 72
4	1E	202/206 (98%)	189 (94%)	12 (6%)	1 (0%)	29 68
4	2E	202/206 (98%)	184 (91%)	15 (7%)	3 (2%)	10 42
5	1F	201/210 (96%)	184 (92%)	16 (8%)	1 (0%)	29 68
5	2F	201/210 (96%)	190 (94%)	10 (5%)	1 (0%)	29 68
6	1G	179/182 (98%)	165 (92%)	10 (6%)	4 (2%)	6 31
6	2G	179/182 (98%)	151 (84%)	26 (14%)	2 (1%)	14 50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
7	1H	172/180 (96%)	149 (87%)	20 (12%)	3 (2%)	9 39
7	2H	172/180 (96%)	156 (91%)	12 (7%)	4 (2%)	6 30
8	1I	144/148 (97%)	129 (90%)	15 (10%)	0	100 100
8	2I	144/148 (97%)	115 (80%)	25 (17%)	4 (3%)	5 25
9	1N	138/140 (99%)	128 (93%)	8 (6%)	2 (1%)	11 43
9	2N	138/140 (99%)	126 (91%)	11 (8%)	1 (1%)	22 60
10	1O	120/122 (98%)	109 (91%)	11 (9%)	0	100 100
10	2O	120/122 (98%)	107 (89%)	12 (10%)	1 (1%)	19 57
11	1P	147/150 (98%)	135 (92%)	10 (7%)	2 (1%)	11 43
11	2P	147/150 (98%)	129 (88%)	18 (12%)	0	100 100
12	1Q	139/141 (99%)	123 (88%)	15 (11%)	1 (1%)	22 60
12	2Q	139/141 (99%)	126 (91%)	12 (9%)	1 (1%)	22 60
13	1R	116/118 (98%)	109 (94%)	5 (4%)	2 (2%)	9 39
13	2R	116/118 (98%)	105 (90%)	10 (9%)	1 (1%)	17 55
14	1S	108/112 (96%)	97 (90%)	10 (9%)	1 (1%)	17 55
14	2S	108/112 (96%)	98 (91%)	8 (7%)	2 (2%)	8 36
15	1T	129/146 (88%)	115 (89%)	11 (8%)	3 (2%)	6 30
15	2T	129/146 (88%)	118 (92%)	10 (8%)	1 (1%)	19 57
16	1U	114/118 (97%)	107 (94%)	7 (6%)	0	100 100
16	2U	114/118 (97%)	108 (95%)	6 (5%)	0	100 100
17	1V	99/101 (98%)	89 (90%)	10 (10%)	0	100 100
17	2V	99/101 (98%)	89 (90%)	9 (9%)	1 (1%)	15 53
18	1W	110/113 (97%)	105 (96%)	3 (3%)	2 (2%)	8 37
18	2W	110/113 (97%)	101 (92%)	9 (8%)	0	100 100
19	1X	93/96 (97%)	85 (91%)	8 (9%)	0	100 100
19	2X	93/96 (97%)	79 (85%)	13 (14%)	1 (1%)	14 50
20	1Y	105/110 (96%)	94 (90%)	9 (9%)	2 (2%)	8 36
20	2Y	105/110 (96%)	90 (86%)	14 (13%)	1 (1%)	15 53
21	1Z	148/206 (72%)	127 (86%)	20 (14%)	1 (1%)	22 60
21	2Z	156/206 (76%)	130 (83%)	24 (15%)	2 (1%)	12 45
22	10	74/85 (87%)	69 (93%)	5 (7%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
22	20	74/85 (87%)	65 (88%)	8 (11%)	1 (1%)	11 43
23	11	95/98 (97%)	92 (97%)	3 (3%)	0	100 100
23	21	95/98 (97%)	90 (95%)	5 (5%)	0	100 100
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100 100
24	22	68/72 (94%)	65 (96%)	2 (3%)	1 (2%)	10 42
25	13	57/60 (95%)	53 (93%)	4 (7%)	0	100 100
25	23	57/60 (95%)	56 (98%)	1 (2%)	0	100 100
26	14	67/71 (94%)	50 (75%)	12 (18%)	5 (8%)	1 5
26	24	67/71 (94%)	48 (72%)	15 (22%)	4 (6%)	1 9
27	15	57/60 (95%)	55 (96%)	2 (4%)	0	100 100
27	25	57/60 (95%)	57 (100%)	0	0	100 100
28	16	51/54 (94%)	50 (98%)	1 (2%)	0	100 100
28	26	51/54 (94%)	49 (96%)	2 (4%)	0	100 100
29	17	46/49 (94%)	44 (96%)	2 (4%)	0	100 100
29	27	46/49 (94%)	44 (96%)	2 (4%)	0	100 100
30	18	62/65 (95%)	59 (95%)	3 (5%)	0	100 100
30	28	62/65 (95%)	58 (94%)	4 (6%)	0	100 100
31	19	35/37 (95%)	35 (100%)	0	0	100 100
31	29	35/37 (95%)	31 (89%)	4 (11%)	0	100 100
33	1b	229/256 (90%)	198 (86%)	24 (10%)	7 (3%)	4 23
33	2b	229/256 (90%)	182 (80%)	38 (17%)	9 (4%)	3 17
34	1c	204/239 (85%)	179 (88%)	23 (11%)	2 (1%)	15 53
34	2c	204/239 (85%)	165 (81%)	33 (16%)	6 (3%)	4 24
35	1d	206/209 (99%)	191 (93%)	15 (7%)	0	100 100
35	2d	206/209 (99%)	183 (89%)	21 (10%)	2 (1%)	15 53
36	1e	146/162 (90%)	130 (89%)	12 (8%)	4 (3%)	5 26
36	2e	146/162 (90%)	130 (89%)	15 (10%)	1 (1%)	22 60
37	1f	98/101 (97%)	85 (87%)	13 (13%)	0	100 100
37	2f	98/101 (97%)	93 (95%)	4 (4%)	1 (1%)	15 53
38	1g	153/156 (98%)	130 (85%)	21 (14%)	2 (1%)	12 45
38	2g	153/156 (98%)	132 (86%)	17 (11%)	4 (3%)	5 27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
39	1h	135/138 (98%)	121 (90%)	14 (10%)	0	100 100
39	2h	135/138 (98%)	121 (90%)	14 (10%)	0	100 100
40	1i	125/128 (98%)	109 (87%)	13 (10%)	3 (2%)	6 29
40	2i	125/128 (98%)	104 (83%)	20 (16%)	1 (1%)	19 57
41	1j	95/105 (90%)	78 (82%)	13 (14%)	4 (4%)	3 16
41	2j	94/105 (90%)	79 (84%)	13 (14%)	2 (2%)	7 33
42	1k	112/129 (87%)	100 (89%)	12 (11%)	0	100 100
42	2k	112/129 (87%)	88 (79%)	19 (17%)	5 (4%)	2 14
43	1l	119/132 (90%)	104 (87%)	15 (13%)	0	100 100
43	2l	119/132 (90%)	103 (87%)	15 (13%)	1 (1%)	19 57
44	1m	121/126 (96%)	106 (88%)	12 (10%)	3 (2%)	5 28
44	2m	120/126 (95%)	96 (80%)	20 (17%)	4 (3%)	4 21
45	1n	58/61 (95%)	49 (84%)	9 (16%)	0	100 100
45	2n	58/61 (95%)	49 (84%)	8 (14%)	1 (2%)	9 39
46	1o	86/89 (97%)	79 (92%)	6 (7%)	1 (1%)	13 48
46	2o	86/89 (97%)	76 (88%)	10 (12%)	0	100 100
47	1p	80/88 (91%)	70 (88%)	9 (11%)	1 (1%)	12 45
47	2p	80/88 (91%)	69 (86%)	10 (12%)	1 (1%)	12 45
48	1q	97/105 (92%)	79 (81%)	18 (19%)	0	100 100
48	2q	97/105 (92%)	85 (88%)	12 (12%)	0	100 100
49	1r	66/88 (75%)	59 (89%)	5 (8%)	2 (3%)	4 24
49	2r	66/88 (75%)	64 (97%)	2 (3%)	0	100 100
50	1s	81/93 (87%)	68 (84%)	13 (16%)	0	100 100
50	2s	81/93 (87%)	63 (78%)	17 (21%)	1 (1%)	13 48
51	1t	94/106 (89%)	79 (84%)	10 (11%)	5 (5%)	2 11
51	2t	94/106 (89%)	82 (87%)	8 (8%)	4 (4%)	2 15
52	1u	21/27 (78%)	19 (90%)	2 (10%)	0	100 100
52	2u	21/27 (78%)	17 (81%)	3 (14%)	1 (5%)	2 13
55	1z	14/16 (88%)	14 (100%)	0	0	100 100
55	2z	14/16 (88%)	14 (100%)	0	0	100 100
All	All	11384/12160 (94%)	10116 (89%)	1126 (10%)	142 (1%)	13 48

All (142) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
7	1H	126	PRO
11	1P	53	GLY
12	1Q	60	ARG
21	1Z	52	SER
26	14	53	GLU
33	1b	125	PRO
33	1b	126	GLU
38	1g	80	VAL
40	1i	54	ASP
41	1j	55	LYS
44	1m	67	GLU
44	1m	106	ASN
5	2F	130	ALA
7	2H	126	PRO
8	2I	10	GLU
20	2Y	16	ALA
26	24	49	PHE
33	2b	17	PHE
33	2b	126	GLU
34	2c	74	GLY
38	2g	80	VAL
42	2k	49	GLY
42	2k	106	LYS
44	2m	67	GLU
51	2t	10	LEU
6	1G	43	LEU
6	1G	126	ASP
11	1P	36	LYS
15	1T	13	ARG
26	14	49	PHE
26	14	62	ARG
33	1b	17	PHE
36	1e	86	ALA
40	1i	56	LEU
41	1j	93	GLY
47	1p	28	ARG
6	2G	51	ARG
6	2G	126	ASP
8	2I	117	GLU
9	2N	2	LYS
10	2O	5	GLN

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Mol	Chain	Res	Type
13	2R	14	SER
14	2S	84	GLN
17	2V	79	VAL
19	2X	93	GLU
33	2b	9	GLU
33	2b	10	LEU
33	2b	123	ALA
34	2c	95	THR
34	2c	145	GLY
41	2j	79	ARG
44	2m	106	ASN
45	2n	14	PRO
50	2s	81	ARG
51	2t	100	ILE
3	1D	256	GLY
7	1H	109	PHE
13	1R	107	ASP
14	1S	94	TYR
18	1W	40	ASN
26	14	45	GLY
33	1b	101	MET
33	1b	231	GLU
36	1e	6	PHE
36	1e	77	PRO
41	1j	77	PRO
41	1j	92	THR
51	1t	10	LEU
21	2Z	93	ASP
26	24	48	ARG
33	2b	74	LYS
33	2b	190	THR
34	2c	4	LYS
34	2c	129	ALA
38	2g	7	ALA
38	2g	153	HIS
42	2k	54	ARG
4	1E	52	LEU
6	1G	49	ASP
6	1G	124	SER
9	1N	111	PRO
13	1R	2	ARG
15	1T	127	ALA

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Mol	Chain	Res	Type
20	1Y	54	LYS
26	14	29	PRO
34	1c	26	LYS
34	1c	156	ARG
38	1g	130	GLY
44	1m	36	LYS
46	1o	19	PRO
49	1r	25	THR
4	2E	52	LEU
4	2E	131	ALA
4	2E	144	ARG
7	2H	47	GLU
7	2H	92	ILE
8	2I	40	THR
12	2Q	13	GLN
15	2T	129	ARG
21	2Z	52	SER
35	2d	42	GLN
35	2d	186	LEU
41	2j	55	LYS
44	2m	36	LYS
47	2p	53	VAL
51	2t	47	GLY
52	2u	3	LYS
9	1N	18	ALA
33	1b	20	GLU
36	1e	85	GLY
40	1i	33	PHE
49	1r	33	ASP
51	1t	47	GLY
3	2D	241	PRO
8	2I	112	LYS
14	2S	79	ALA
22	20	83	PRO
26	24	62	ARG
33	2b	131	PRO
43	2l	45	PRO
51	2t	95	ALA
15	1T	128	GLU
18	1W	111	HIS
20	1Y	53	PRO
51	1t	96	GLY

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Mol	Chain	Res	Type
24	22	18	PRO
26	24	3	GLU
34	2c	73	PRO
44	2m	35	GLU
42	2k	118	GLY
33	1b	124	SER
51	1t	102	GLY
33	2b	165	VAL
37	2f	40	VAL
42	2k	34	ASP
7	1H	118	PRO
7	2H	55	PRO
40	2i	53	VAL
38	2g	17	VAL
51	1t	100	ILE
36	2e	77	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%)	193 (90%)	22 (10%)	7 28
3	2D	215/218 (99%)	186 (86%)	29 (14%)	4 17
4	1E	164/166 (99%)	150 (92%)	14 (8%)	10 38
4	2E	164/166 (99%)	148 (90%)	16 (10%)	8 30
5	1F	160/166 (96%)	148 (92%)	12 (8%)	13 43
5	2F	159/166 (96%)	145 (91%)	14 (9%)	10 36
6	1G	143/156 (92%)	128 (90%)	15 (10%)	7 27
6	2G	143/156 (92%)	132 (92%)	11 (8%)	13 42
7	1H	144/148 (97%)	132 (92%)	12 (8%)	11 39
7	2H	144/148 (97%)	132 (92%)	12 (8%)	11 39
8	1I	113/124 (91%)	99 (88%)	14 (12%)	4 20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	2I	105/124 (85%)	92 (88%)	13 (12%)	4 20
9	1N	118/119 (99%)	107 (91%)	11 (9%)	9 33
9	2N	118/119 (99%)	104 (88%)	14 (12%)	5 22
10	1O	100/100 (100%)	92 (92%)	8 (8%)	12 40
10	2O	100/100 (100%)	92 (92%)	8 (8%)	12 40
11	1P	115/116 (99%)	101 (88%)	14 (12%)	5 21
11	2P	115/116 (99%)	103 (90%)	12 (10%)	7 27
12	1Q	111/111 (100%)	104 (94%)	7 (6%)	18 51
12	2Q	111/111 (100%)	98 (88%)	13 (12%)	5 22
13	1R	101/101 (100%)	87 (86%)	14 (14%)	3 16
13	2R	101/101 (100%)	91 (90%)	10 (10%)	8 30
14	1S	86/88 (98%)	76 (88%)	10 (12%)	5 23
14	2S	85/88 (97%)	77 (91%)	8 (9%)	8 32
15	1T	115/127 (91%)	111 (96%)	4 (4%)	36 71
15	2T	113/127 (89%)	104 (92%)	9 (8%)	12 40
16	1U	93/94 (99%)	85 (91%)	8 (9%)	10 37
16	2U	93/94 (99%)	86 (92%)	7 (8%)	13 43
17	1V	80/82 (98%)	71 (89%)	9 (11%)	6 24
17	2V	80/82 (98%)	74 (92%)	6 (8%)	13 43
18	1W	90/92 (98%)	85 (94%)	5 (6%)	21 56
18	2W	90/92 (98%)	85 (94%)	5 (6%)	21 56
19	1X	77/78 (99%)	73 (95%)	4 (5%)	23 59
19	2X	77/78 (99%)	74 (96%)	3 (4%)	32 69
20	1Y	85/91 (93%)	77 (91%)	8 (9%)	8 32
20	2Y	85/91 (93%)	74 (87%)	11 (13%)	4 19
21	1Z	135/179 (75%)	122 (90%)	13 (10%)	8 32
21	2Z	137/179 (76%)	113 (82%)	24 (18%)	2 10
22	10	61/67 (91%)	58 (95%)	3 (5%)	25 61
22	20	61/67 (91%)	56 (92%)	5 (8%)	11 39
23	11	80/83 (96%)	77 (96%)	3 (4%)	33 69
23	21	80/83 (96%)	76 (95%)	4 (5%)	24 60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
24	12	65/67 (97%)	59 (91%)	6 (9%)	9 34
24	22	65/67 (97%)	61 (94%)	4 (6%)	18 52
25	13	51/52 (98%)	45 (88%)	6 (12%)	5 22
25	23	50/52 (96%)	47 (94%)	3 (6%)	19 53
26	14	59/63 (94%)	52 (88%)	7 (12%)	5 22
26	24	53/63 (84%)	48 (91%)	5 (9%)	8 32
27	15	50/52 (96%)	44 (88%)	6 (12%)	5 22
27	25	50/52 (96%)	46 (92%)	4 (8%)	12 40
28	16	51/52 (98%)	43 (84%)	8 (16%)	2 13
28	26	50/52 (96%)	41 (82%)	9 (18%)	1 9
29	17	41/42 (98%)	37 (90%)	4 (10%)	8 30
29	27	41/42 (98%)	33 (80%)	8 (20%)	1 7
30	18	54/55 (98%)	50 (93%)	4 (7%)	13 44
30	28	54/55 (98%)	49 (91%)	5 (9%)	9 33
31	19	34/34 (100%)	32 (94%)	2 (6%)	19 54
31	29	34/34 (100%)	30 (88%)	4 (12%)	5 22
33	1b	192/220 (87%)	171 (89%)	21 (11%)	6 25
33	2b	187/220 (85%)	162 (87%)	25 (13%)	4 17
34	1c	142/188 (76%)	130 (92%)	12 (8%)	10 38
34	2c	140/188 (74%)	120 (86%)	20 (14%)	3 15
35	1d	169/181 (93%)	149 (88%)	20 (12%)	5 22
35	2d	173/181 (96%)	161 (93%)	12 (7%)	15 48
36	1e	113/123 (92%)	103 (91%)	10 (9%)	10 36
36	2e	114/123 (93%)	103 (90%)	11 (10%)	8 32
37	1f	84/90 (93%)	76 (90%)	8 (10%)	8 32
37	2f	85/90 (94%)	75 (88%)	10 (12%)	5 22
38	1g	119/127 (94%)	113 (95%)	6 (5%)	24 60
38	2g	120/127 (94%)	111 (92%)	9 (8%)	13 43
39	1h	114/119 (96%)	104 (91%)	10 (9%)	10 36
39	2h	114/119 (96%)	107 (94%)	7 (6%)	18 53
40	1i	90/99 (91%)	77 (86%)	13 (14%)	3 15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
40	2i	89/99 (90%)	78 (88%)	11 (12%)	4 20
41	1j	66/92 (72%)	58 (88%)	8 (12%)	5 21
41	2j	69/92 (75%)	62 (90%)	7 (10%)	7 29
42	1k	82/99 (83%)	74 (90%)	8 (10%)	8 30
42	2k	83/99 (84%)	74 (89%)	9 (11%)	6 26
43	1l	96/108 (89%)	90 (94%)	6 (6%)	18 51
43	2l	96/108 (89%)	88 (92%)	8 (8%)	11 39
44	1m	93/101 (92%)	83 (89%)	10 (11%)	6 26
44	2m	92/101 (91%)	83 (90%)	9 (10%)	8 30
45	1n	49/50 (98%)	41 (84%)	8 (16%)	2 11
45	2n	49/50 (98%)	42 (86%)	7 (14%)	3 15
46	1o	78/80 (98%)	73 (94%)	5 (6%)	17 51
46	2o	78/80 (98%)	67 (86%)	11 (14%)	3 16
47	1p	69/74 (93%)	62 (90%)	7 (10%)	7 29
47	2p	68/74 (92%)	59 (87%)	9 (13%)	4 18
48	1q	94/97 (97%)	86 (92%)	8 (8%)	10 38
48	2q	94/97 (97%)	88 (94%)	6 (6%)	17 51
49	1r	59/77 (77%)	56 (95%)	3 (5%)	24 60
49	2r	59/77 (77%)	52 (88%)	7 (12%)	5 22
50	1s	69/80 (86%)	66 (96%)	3 (4%)	29 66
50	2s	67/80 (84%)	59 (88%)	8 (12%)	5 22
51	1t	70/82 (85%)	63 (90%)	7 (10%)	7 29
51	2t	70/82 (85%)	64 (91%)	6 (9%)	10 37
52	1u	18/22 (82%)	17 (94%)	1 (6%)	21 56
52	2u	18/22 (82%)	18 (100%)	0	100 100
55	1z	15/16 (94%)	14 (93%)	1 (7%)	16 49
55	2z	15/16 (94%)	13 (87%)	2 (13%)	4 17
All	All	9325/10096 (92%)	8427 (90%)	898 (10%)	8 32

All (898) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	3	VAL

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Mol	Chain	Res	Type
3	1D	12	SER
3	1D	13	ARG
3	1D	22	SER
3	1D	32	SER
3	1D	71	ASP
3	1D	88	ARG
3	1D	106	ILE
3	1D	115	GLN
3	1D	122	ASP
3	1D	141	VAL
3	1D	142	VAL
3	1D	181	GLU
3	1D	182	LEU
3	1D	193	VAL
3	1D	211	ARG
3	1D	221	VAL
3	1D	229	VAL
3	1D	230	ASP
3	1D	237	GLU
3	1D	242	ARG
3	1D	261	LYS
4	1E	9	VAL
4	1E	12	THR
4	1E	21	VAL
4	1E	24	THR
4	1E	47	VAL
4	1E	51	PHE
4	1E	73	GLU
4	1E	75	VAL
4	1E	89	ASP
4	1E	116	VAL
4	1E	149	ARG
4	1E	160	TYR
4	1E	181	LEU
4	1E	184	VAL
5	1F	13	SER
5	1F	17	ARG
5	1F	53	THR
5	1F	57	VAL
5	1F	60	SER
5	1F	64	ILE
5	1F	74	ARG

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Mol	Chain	Res	Type
5	1F	158	THR
5	1F	170	LEU
5	1F	192	LEU
5	1F	195	ASP
5	1F	197	ASP
6	1G	3	LEU
6	1G	4	ASP
6	1G	14	GLU
6	1G	21	ARG
6	1G	28	VAL
6	1G	43	LEU
6	1G	62	LEU
6	1G	70	VAL
6	1G	79	ASN
6	1G	133	LEU
6	1G	139	LEU
6	1G	140	ILE
6	1G	148	MET
6	1G	149	VAL
6	1G	170	ARG
7	1H	13	LYS
7	1H	18	GLU
7	1H	45	VAL
7	1H	46	GLU
7	1H	49	VAL
7	1H	56	SER
7	1H	71	LEU
7	1H	111	HIS
7	1H	114	VAL
7	1H	129	THR
7	1H	134	SER
7	1H	169	VAL
8	1I	12	LEU
8	1I	40	THR
8	1I	47	LEU
8	1I	68	LEU
8	1I	75	LEU
8	1I	76	THR
8	1I	92	VAL
8	1I	96	ASP
8	1I	101	LEU
8	1I	109	ILE

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Mol	Chain	Res	Type
8	1I	117	GLU
8	1I	128	LEU
8	1I	140	LEU
8	1I	142	VAL
9	1N	5	VAL
9	1N	28	THR
9	1N	33	LEU
9	1N	46	VAL
9	1N	67	LEU
9	1N	71	ILE
9	1N	85	ILE
9	1N	87	LEU
9	1N	89	LYS
9	1N	96	GLU
9	1N	114	ARG
10	1O	10	VAL
10	1O	13	ASN
10	1O	21	CYS
10	1O	64	ARG
10	1O	66	LYS
10	1O	80	ASP
10	1O	96	THR
10	1O	114	ILE
11	1P	3	LEU
11	1P	4	SER
11	1P	29	LYS
11	1P	57	THR
11	1P	61	ARG
11	1P	65	ARG
11	1P	83	VAL
11	1P	95	VAL
11	1P	96	THR
11	1P	98	GLU
11	1P	125	VAL
11	1P	126	VAL
11	1P	136	GLU
11	1P	147	LEU
12	1Q	27	VAL
12	1Q	56	ARG
12	1Q	60	ARG
12	1Q	63	LYS
12	1Q	110	THR

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Mol	Chain	Res	Type
12	1Q	129	THR
12	1Q	133	ARG
13	1R	1	MET
13	1R	6	SER
13	1R	27	SER
13	1R	33	ARG
13	1R	36	THR
13	1R	44	LEU
13	1R	54	LEU
13	1R	65	LEU
13	1R	67	LEU
13	1R	79	LEU
13	1R	98	LEU
13	1R	104	ARG
13	1R	111	LEU
13	1R	114	VAL
14	1S	4	LEU
14	1S	14	VAL
14	1S	36	TYR
14	1S	38	GLN
14	1S	42	ASP
14	1S	50	SER
14	1S	56	LEU
14	1S	63	THR
14	1S	69	VAL
14	1S	98	VAL
15	1T	28	VAL
15	1T	96	ARG
15	1T	108	ARG
15	1T	128	GLU
16	1U	8	VAL
16	1U	31	SER
16	1U	59	ARG
16	1U	70	ARG
16	1U	74	LEU
16	1U	83	LEU
16	1U	95	LEU
16	1U	117	GLN
17	1V	32	THR
17	1V	49	THR
17	1V	52	VAL
17	1V	62	LEU

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Mol	Chain	Res	Type
17	1V	72	VAL
17	1V	79	VAL
17	1V	82	ARG
17	1V	90	PRO
17	1V	100	ARG
18	1W	15	ARG
18	1W	17	VAL
18	1W	23	LEU
18	1W	72	LYS
18	1W	107	LEU
19	1X	5	TYR
19	1X	30	VAL
19	1X	65	ARG
19	1X	70	LEU
20	1Y	5	MET
20	1Y	6	HIS
20	1Y	7	VAL
20	1Y	45	VAL
20	1Y	55	TYR
20	1Y	72	VAL
20	1Y	99	CYS
20	1Y	107	ASP
21	1Z	28	MET
21	1Z	31	ARG
21	1Z	33	LEU
21	1Z	37	VAL
21	1Z	52	SER
21	1Z	61	LEU
21	1Z	86	VAL
21	1Z	91	LEU
21	1Z	93	ASP
21	1Z	141	VAL
21	1Z	148	ASP
21	1Z	154	ASP
21	1Z	155	LEU
22	10	14	ARG
22	10	37	LEU
22	10	43	THR
23	11	38	SER
23	11	56	GLN
23	11	95	LEU
24	12	1	MET

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Mol	Chain	Res	Type
24	12	5	GLU
24	12	19	VAL
24	12	30	ARG
24	12	53	LEU
24	12	57	ILE
25	13	6	VAL
25	13	23	LEU
25	13	57	GLU
25	13	58	VAL
25	13	59	VAL
25	13	60	GLU
26	14	1	MET
26	14	27	THR
26	14	49	PHE
26	14	59	PHE
26	14	61	ARG
26	14	63	TYR
26	14	67	TYR
27	15	6	VAL
27	15	16	ARG
27	15	26	THR
27	15	29	THR
27	15	58	LEU
27	15	59	GLU
28	16	6	ARG
28	16	9	LEU
28	16	13	CYS
28	16	19	ARG
28	16	40	CYS
28	16	44	ARG
28	16	47	THR
28	16	48	VAL
29	17	1	MET
29	17	41	ARG
29	17	42	LEU
29	17	47	ARG
30	18	6	THR
30	18	29	LYS
30	18	31	HIS
30	18	34	TRP
31	19	7	VAL
31	19	26	ILE

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Mol	Chain	Res	Type
33	1b	19	HIS
33	1b	30	ARG
33	1b	44	LEU
33	1b	52	GLU
33	1b	53	ARG
33	1b	59	GLU
33	1b	80	ILE
33	1b	81	VAL
33	1b	93	VAL
33	1b	96	ARG
33	1b	112	VAL
33	1b	128	GLU
33	1b	142	LEU
33	1b	156	LYS
33	1b	160	ASP
33	1b	185	ILE
33	1b	198	ASP
33	1b	200	ILE
33	1b	211	ILE
33	1b	217	ARG
33	1b	223	ILE
34	1c	8	ILE
34	1c	15	THR
34	1c	17	ASP
34	1c	28	GLN
34	1c	29	TYR
34	1c	46	GLU
34	1c	47	LEU
34	1c	64	VAL
34	1c	132	ARG
34	1c	144	SER
34	1c	191	THR
34	1c	202	ILE
35	1d	3	ARG
35	1d	19	LEU
35	1d	21	LEU
35	1d	52	SER
35	1d	53	ASP
35	1d	59	ARG
35	1d	83	SER
35	1d	127	THR
35	1d	134	ASP

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Mol	Chain	Res	Type
35	1d	135	LEU
35	1d	152	SER
35	1d	156	GLU
35	1d	157	LEU
35	1d	158	ILE
35	1d	165	MET
35	1d	176	LEU
35	1d	178	VAL
35	1d	182	LYS
35	1d	193	ASP
35	1d	200	GLU
36	1e	12	LEU
36	1e	20	GLN
36	1e	34	VAL
36	1e	38	GLN
36	1e	41	VAL
36	1e	53	LEU
36	1e	76	ILE
36	1e	81	GLU
36	1e	91	LEU
36	1e	120	THR
37	1f	25	ILE
37	1f	37	VAL
37	1f	43	LEU
37	1f	59	TYR
37	1f	72	VAL
37	1f	73	ASN
37	1f	75	LEU
37	1f	78	GLU
38	1g	13	GLN
38	1g	16	LEU
38	1g	24	THR
38	1g	35	LYS
38	1g	50	ILE
38	1g	113	GLU
39	1h	25	ASP
39	1h	29	SER
39	1h	51	VAL
39	1h	63	LEU
39	1h	68	ARG
39	1h	84	ARG
39	1h	85	ARG

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Mol	Chain	Res	Type
39	1h	91	ARG
39	1h	104	ARG
39	1h	107	LEU
40	1i	20	ARG
40	1i	51	ARG
40	1i	53	VAL
40	1i	64	THR
40	1i	70	LYS
40	1i	81	ILE
40	1i	92	TYR
40	1i	96	LEU
40	1i	104	ARG
40	1i	108	VAL
40	1i	111	ARG
40	1i	113	LYS
40	1i	117	HIS
41	1j	16	LEU
41	1j	17	ASP
41	1j	34	VAL
41	1j	44	VAL
41	1j	55	LYS
41	1j	81	THR
41	1j	85	LEU
41	1j	100	THR
42	1k	26	ASN
42	1k	31	THR
42	1k	38	ASN
42	1k	48	ILE
42	1k	87	THR
42	1k	104	GLN
42	1k	105	VAL
42	1k	109	VAL
43	1l	54	LYS
43	1l	67	THR
43	1l	70	ILE
43	1l	83	VAL
43	1l	86	ARG
43	1l	118	SER
44	1m	4	ILE
44	1m	11	ARG
44	1m	17	VAL
44	1m	43	THR

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Mol	Chain	Res	Type
44	1m	49	THR
44	1m	63	THR
44	1m	103	THR
44	1m	109	THR
44	1m	110	ARG
44	1m	116	THR
45	1n	3	ARG
45	1n	13	THR
45	1n	18	VAL
45	1n	22	THR
45	1n	33	VAL
45	1n	35	ARG
45	1n	41	ARG
45	1n	56	VAL
46	1o	5	LYS
46	1o	6	GLU
46	1o	11	VAL
46	1o	14	GLU
46	1o	83	GLU
47	1p	11	SER
47	1p	20	VAL
47	1p	29	ASP
47	1p	33	ILE
47	1p	45	THR
47	1p	67	THR
47	1p	72	ARG
48	1q	11	VAL
48	1q	35	VAL
48	1q	37	LYS
48	1q	59	ILE
48	1q	60	ILE
48	1q	63	ARG
48	1q	70	ARG
48	1q	72	ARG
49	1r	21	LYS
49	1r	42	ARG
49	1r	76	LEU
50	1s	5	LEU
50	1s	71	LEU
50	1s	79	THR
51	1t	9	ASN
51	1t	10	LEU

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Mol	Chain	Res	Type
51	1t	20	LEU
51	1t	24	LEU
51	1t	37	SER
51	1t	56	MET
51	1t	63	ILE
52	1u	17	THR
55	1z	6	ARG
3	2D	3	VAL
3	2D	10	THR
3	2D	14	ARG
3	2D	25	THR
3	2D	54	ARG
3	2D	69	ARG
3	2D	71	ASP
3	2D	72	LYS
3	2D	83	GLU
3	2D	88	ARG
3	2D	94	LEU
3	2D	111	LEU
3	2D	131	LEU
3	2D	134	ARG
3	2D	141	VAL
3	2D	157	ARG
3	2D	169	GLU
3	2D	171	ASP
3	2D	182	LEU
3	2D	193	VAL
3	2D	211	ARG
3	2D	217	ARG
3	2D	222	ARG
3	2D	229	VAL
3	2D	237	GLU
3	2D	242	ARG
3	2D	253	GLN
3	2D	259	THR
3	2D	276	LYS
4	2E	1	MET
4	2E	9	VAL
4	2E	17	ASP
4	2E	24	THR
4	2E	38	THR
4	2E	42	ASP

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Mol	Chain	Res	Type
4	2E	52	LEU
4	2E	58	ARG
4	2E	75	VAL
4	2E	83	ASP
4	2E	102	VAL
4	2E	105	THR
4	2E	116	VAL
4	2E	181	LEU
4	2E	182	LEU
4	2E	195	LEU
5	2F	11	VAL
5	2F	17	ARG
5	2F	20	LEU
5	2F	33	LEU
5	2F	88	VAL
5	2F	89	VAL
5	2F	98	SER
5	2F	110	LEU
5	2F	135	LYS
5	2F	145	GLU
5	2F	153	SER
5	2F	158	THR
5	2F	170	LEU
5	2F	192	LEU
6	2G	5	VAL
6	2G	28	VAL
6	2G	38	VAL
6	2G	43	LEU
6	2G	51	ARG
6	2G	60	LEU
6	2G	79	ASN
6	2G	111	LEU
6	2G	140	ILE
6	2G	145	THR
6	2G	155	MET
7	2H	43	VAL
7	2H	45	VAL
7	2H	67	LEU
7	2H	70	THR
7	2H	99	VAL
7	2H	105	LEU
7	2H	106	THR

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Mol	Chain	Res	Type
7	2H	119	GLU
7	2H	122	THR
7	2H	130	ARG
7	2H	134	SER
7	2H	136	ILE
8	2I	3	VAL
8	2I	15	VAL
8	2I	38	LEU
8	2I	61	ARG
8	2I	81	VAL
8	2I	87	LYS
8	2I	92	VAL
8	2I	101	LEU
8	2I	102	SER
8	2I	127	VAL
8	2I	129	THR
8	2I	140	LEU
8	2I	144	VAL
9	2N	14	VAL
9	2N	21	LYS
9	2N	22	THR
9	2N	33	LEU
9	2N	34	LEU
9	2N	43	THR
9	2N	46	VAL
9	2N	62	VAL
9	2N	73	THR
9	2N	76	SER
9	2N	85	ILE
9	2N	90	MET
9	2N	99	LEU
9	2N	112	LEU
10	2O	3	GLN
10	2O	5	GLN
10	2O	17	ARG
10	2O	70	LYS
10	2O	75	SER
10	2O	89	ASN
10	2O	92	GLU
10	2O	105	GLU
11	2P	5	ASP
11	2P	6	LEU

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Mol	Chain	Res	Type
11	2P	29	LYS
11	2P	45	LEU
11	2P	56	SER
11	2P	57	THR
11	2P	86	LYS
11	2P	95	VAL
11	2P	96	THR
11	2P	146	VAL
11	2P	147	LEU
11	2P	148	LEU
12	2Q	1	MET
12	2Q	3	MET
12	2Q	5	ARG
12	2Q	7	MET
12	2Q	16	ARG
12	2Q	25	ASP
12	2Q	38	GLU
12	2Q	55	VAL
12	2Q	60	ARG
12	2Q	98	LYS
12	2Q	106	VAL
12	2Q	109	VAL
12	2Q	135	ASP
13	2R	6	SER
13	2R	15	SER
13	2R	28	LEU
13	2R	29	LEU
13	2R	37	THR
13	2R	44	LEU
13	2R	59	ASP
13	2R	94	TYR
13	2R	95	THR
13	2R	118	GLU
14	2S	8	GLU
14	2S	17	ARG
14	2S	21	THR
14	2S	36	TYR
14	2S	48	LEU
14	2S	52	SER
14	2S	58	LEU
14	2S	101	LEU
15	2T	6	LEU

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Mol	Chain	Res	Type
15	2T	15	VAL
15	2T	16	ARG
15	2T	49	VAL
15	2T	63	VAL
15	2T	64	ARG
15	2T	104	ASN
15	2T	107	ASP
15	2T	125	ARG
16	2U	30	LYS
16	2U	31	SER
16	2U	34	LYS
16	2U	74	LEU
16	2U	98	LEU
16	2U	111	GLU
16	2U	112	ARG
17	2V	7	THR
17	2V	43	GLU
17	2V	46	VAL
17	2V	52	VAL
17	2V	79	VAL
17	2V	82	ARG
18	2W	11	ARG
18	2W	17	VAL
18	2W	39	THR
18	2W	68	ARG
18	2W	71	VAL
19	2X	40	LYS
19	2X	43	VAL
19	2X	57	LEU
20	2Y	6	HIS
20	2Y	9	LYS
20	2Y	30	VAL
20	2Y	40	GLU
20	2Y	44	ILE
20	2Y	49	VAL
20	2Y	61	ILE
20	2Y	64	GLU
20	2Y	66	PRO
20	2Y	85	VAL
20	2Y	96	ILE
21	2Z	5	LEU
21	2Z	24	LEU

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Mol	Chain	Res	Type
21	2Z	27	VAL
21	2Z	28	MET
21	2Z	35	ARG
21	2Z	56	VAL
21	2Z	70	LEU
21	2Z	91	LEU
21	2Z	121	HIS
21	2Z	124	ILE
21	2Z	128	VAL
21	2Z	129	SER
21	2Z	131	ARG
21	2Z	136	PHE
21	2Z	138	GLU
21	2Z	141	VAL
21	2Z	144	LEU
21	2Z	150	LEU
21	2Z	153	SER
21	2Z	154	ASP
21	2Z	161	VAL
21	2Z	170	THR
21	2Z	171	ILE
21	2Z	174	VAL
22	20	10	THR
22	20	29	GLN
22	20	53	MET
22	20	55	ARG
22	20	68	GLU
23	21	4	VAL
23	21	20	ARG
23	21	67	ILE
23	21	82	LEU
24	22	45	SER
24	22	52	ASP
24	22	53	LEU
24	22	64	LEU
25	23	30	ARG
25	23	34	GLU
25	23	57	GLU
26	24	26	SER
26	24	31	ILE
26	24	59	PHE
26	24	63	TYR

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Mol	Chain	Res	Type
26	24	67	TYR
27	25	29	THR
27	25	40	LYS
27	25	48	GLU
27	25	58	LEU
28	26	5	VAL
28	26	13	CYS
28	26	14	THR
28	26	15	GLU
28	26	23	THR
28	26	34	LEU
28	26	49	HIS
28	26	50	ARG
28	26	51	GLU
29	27	1	MET
29	27	4	THR
29	27	15	THR
29	27	24	THR
29	27	39	ARG
29	27	41	ARG
29	27	47	ARG
29	27	48	LYS
30	28	6	THR
30	28	31	HIS
30	28	37	SER
30	28	41	ILE
30	28	56	GLU
31	29	6	SER
31	29	7	VAL
31	29	11	CYS
31	29	12	ASP
33	2b	8	LYS
33	2b	11	LEU
33	2b	16	HIS
33	2b	17	PHE
33	2b	24	TRP
33	2b	35	GLU
33	2b	43	ASP
33	2b	60	ASP
33	2b	67	THR
33	2b	71	VAL
33	2b	78	GLN

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Mol	Chain	Res	Type
33	2b	81	VAL
33	2b	93	VAL
33	2b	94	ASN
33	2b	96	ARG
33	2b	115	LEU
33	2b	124	SER
33	2b	135	GLN
33	2b	139	LYS
33	2b	164	VAL
33	2b	166	ASP
33	2b	179	LYS
33	2b	204	ASN
33	2b	208	ILE
33	2b	235	SER
34	2c	15	THR
34	2c	20	SER
34	2c	21	ARG
34	2c	36	ASP
34	2c	47	LEU
34	2c	49	SER
34	2c	55	VAL
34	2c	70	VAL
34	2c	91	LEU
34	2c	103	VAL
34	2c	105	GLU
34	2c	131	ARG
34	2c	152	ILE
34	2c	154	SER
34	2c	162	GLN
34	2c	164	ARG
34	2c	190	ARG
34	2c	193	TYR
34	2c	195	VAL
34	2c	198	VAL
35	2d	12	CYS
35	2d	31	CYS
35	2d	34	GLU
35	2d	76	ARG
35	2d	78	LEU
35	2d	86	LYS
35	2d	122	ARG
35	2d	127	THR

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Mol	Chain	Res	Type
35	2d	135	LEU
35	2d	144	ASP
35	2d	194	LEU
35	2d	196	LEU
36	2e	9	LYS
36	2e	11	ILE
36	2e	13	ILE
36	2e	14	ARG
36	2e	25	ARG
36	2e	31	LEU
36	2e	55	VAL
36	2e	72	GLN
36	2e	76	ILE
36	2e	81	GLU
36	2e	90	VAL
37	2f	10	LEU
37	2f	19	LEU
37	2f	31	GLU
37	2f	45	LEU
37	2f	48	LEU
37	2f	78	GLU
37	2f	82	ARG
37	2f	83	ASP
37	2f	93	SER
37	2f	95	GLU
38	2g	6	ARG
38	2g	9	VAL
38	2g	16	LEU
38	2g	57	GLU
38	2g	79	ARG
38	2g	113	GLU
38	2g	115	ARG
38	2g	119	ARG
38	2g	155	ARG
39	2h	10	LEU
39	2h	45	ILE
39	2h	84	ARG
39	2h	99	GLU
39	2h	104	ARG
39	2h	107	LEU
39	2h	137	VAL
40	2i	19	LEU

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Mol	Chain	Res	Type
40	2i	26	VAL
40	2i	50	LEU
40	2i	53	VAL
40	2i	56	LEU
40	2i	87	GLN
40	2i	88	TYR
40	2i	89	ASN
40	2i	104	ARG
40	2i	108	VAL
40	2i	113	LYS
41	2j	8	LEU
41	2j	15	THR
41	2j	21	GLN
41	2j	40	LEU
41	2j	51	ARG
41	2j	72	VAL
41	2j	89	ASP
42	2k	14	VAL
42	2k	25	TYR
42	2k	41	THR
42	2k	63	LEU
42	2k	87	THR
42	2k	95	ILE
42	2k	105	VAL
42	2k	111	ASP
42	2k	114	VAL
43	2l	6	THR
43	2l	27	LEU
43	2l	36	VAL
43	2l	40	VAL
43	2l	55	VAL
43	2l	86	ARG
43	2l	117	ARG
43	2l	123	LYS
44	2m	11	ARG
44	2m	21	TYR
44	2m	37	THR
44	2m	47	ASP
44	2m	67	GLU
44	2m	91	ARG
44	2m	98	VAL
44	2m	103	THR

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Mol	Chain	Res	Type
44	2m	104	ARG
45	2n	3	ARG
45	2n	6	LEU
45	2n	18	VAL
45	2n	22	THR
45	2n	33	VAL
45	2n	41	ARG
45	2n	46	GLU
46	2o	3	ILE
46	2o	4	THR
46	2o	5	LYS
46	2o	14	GLU
46	2o	24	SER
46	2o	25	THR
46	2o	27	VAL
46	2o	35	ARG
46	2o	83	GLU
46	2o	84	LYS
46	2o	87	ILE
47	2p	2	VAL
47	2p	20	VAL
47	2p	21	VAL
47	2p	22	THR
47	2p	29	ASP
47	2p	42	ARG
47	2p	53	VAL
47	2p	62	VAL
47	2p	67	THR
48	2q	7	THR
48	2q	60	ILE
48	2q	68	ARG
48	2q	79	SER
48	2q	83	ASP
48	2q	96	GLU
49	2r	28	GLU
49	2r	29	PHE
49	2r	47	THR
49	2r	54	ARG
49	2r	65	ILE
49	2r	66	LEU
49	2r	69	THR
50	2s	16	LEU

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Mol	Chain	Res	Type
50	2s	27	GLU
50	2s	28	LYS
50	2s	30	LEU
50	2s	31	ILE
50	2s	33	THR
50	2s	35	SER
50	2s	49	ILE
51	2t	31	SER
51	2t	56	MET
51	2t	62	LEU
51	2t	71	THR
51	2t	72	LEU
51	2t	99	LEU
55	2z	1	TRP
55	2z	9	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (120) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	116	GLN
3	1D	201	HIS
4	1E	48	GLN
5	1F	69	HIS
5	1F	203	GLN
6	1G	26	GLN
6	1G	123	ASN
10	1O	3	GLN
10	1O	90	GLN
12	1Q	57	HIS
12	1Q	89	ASN
12	1Q	123	HIS
15	1T	58	ASN
16	1U	81	HIS
19	1X	31	HIS
20	1Y	6	HIS
20	1Y	43	ASN
21	1Z	32	HIS
21	1Z	54	HIS
21	1Z	73	GLN
22	10	12	ASN
22	10	17	GLN
23	11	19	GLN

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Mol	Chain	Res	Type
23	11	56	GLN
24	12	38	GLN
24	12	70	GLN
27	15	23	HIS
33	1b	16	HIS
33	1b	40	HIS
34	1c	6	HIS
34	1c	28	GLN
34	1c	37	GLN
34	1c	69	HIS
34	1c	162	GLN
34	1c	176	HIS
35	1d	77	ASN
35	1d	116	GLN
35	1d	123	HIS
35	1d	125	HIS
35	1d	201	GLN
36	1e	20	GLN
36	1e	78	HIS
37	1f	7	ASN
37	1f	73	ASN
37	1f	100	ASN
38	1g	13	GLN
38	1g	28	ASN
38	1g	51	GLN
38	1g	106	GLN
40	1i	3	GLN
40	1i	34	ASN
40	1i	58	HIS
40	1i	73	GLN
40	1i	89	ASN
40	1i	117	HIS
40	1i	124	GLN
41	1j	56	HIS
43	1l	80	HIS
44	1m	77	ASN
46	1o	46	HIS
47	1p	13	HIS
47	1p	16	HIS
48	1q	16	GLN
50	1s	57	HIS
3	2D	96	HIS

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Mol	Chain	Res	Type
3	2D	112	GLN
4	2E	48	GLN
4	2E	192	ASN
5	2F	133	ASN
6	2G	132	ASN
10	2O	3	GLN
10	2O	5	GLN
10	2O	89	ASN
11	2P	35	HIS
11	2P	81	GLN
12	2Q	12	GLN
12	2Q	123	HIS
14	2S	38	GLN
14	2S	68	GLN
15	2T	38	ASN
15	2T	58	ASN
15	2T	123	GLN
16	2U	81	HIS
16	2U	94	ASN
19	2X	31	HIS
20	2Y	43	ASN
21	2Z	34	ASN
29	27	6	GLN
31	29	36	GLN
33	2b	40	HIS
33	2b	94	ASN
33	2b	113	HIS
33	2b	212	GLN
34	2c	6	HIS
34	2c	37	GLN
34	2c	123	GLN
34	2c	170	GLN
35	2d	77	ASN
35	2d	116	GLN
35	2d	123	HIS
35	2d	125	HIS
35	2d	160	GLN
36	2e	78	HIS
37	2f	73	ASN
38	2g	109	ASN
38	2g	148	ASN
40	2i	29	ASN

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Mol	Chain	Res	Type
40	2i	89	ASN
41	2j	13	HIS
41	2j	21	GLN
41	2j	62	HIS
42	2k	93	GLN
44	2m	12	ASN
44	2m	77	ASN
50	2s	23	ASN
50	2s	47	HIS
50	2s	57	HIS
50	2s	69	HIS
50	2s	83	HIS
51	2t	9	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2861/2915 (98%)	499 (17%)	29 (1%)
1	2A	2788/2915 (95%)	526 (18%)	21 (0%)
2	1B	120/121 (99%)	14 (11%)	1 (0%)
2	2B	118/121 (97%)	31 (26%)	0
32	1a	1494/1521 (98%)	277 (18%)	0
32	2a	1498/1521 (98%)	270 (18%)	0
53	1v	12/24 (50%)	6 (50%)	0
53	2v	12/24 (50%)	4 (33%)	0
54	1x	75/77 (97%)	11 (14%)	0
54	2x	75/77 (97%)	13 (17%)	0
All	All	9053/9316 (97%)	1651 (18%)	51 (0%)

All (1651) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	13	A
1	1A	34	C
1	1A	36	G
1	1A	45	C
1	1A	55	G
1	1A	58	G
1	1A	64	A
1	1A	71	A

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Mol	Chain	Res	Type
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	154	G
1	1A	182	A
1	1A	196	A
1	1A	198	C
1	1A	199	A
1	1A	201	C
1	1A	205	G
1	1A	214	G
1	1A	216	A
1	1A	221	A
1	1A	222	A
1	1A	228	A
1	1A	229	A
1	1A	230	U
1	1A	233	A
1	1A	248	G
1	1A	249	C
1	1A	269	U
1	1A	271(C)	C
1	1A	271(E)	U
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	271(S)	G
1	1A	272(B)	G
1	1A	279	C
1	1A	294	A
1	1A	311	A
1	1A	329	G
1	1A	330	A
1	1A	331	A
1	1A	338	G

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Mol	Chain	Res	Type
1	1A	346	A
1	1A	352	G
1	1A	362	U
1	1A	363	G
1	1A	363(B)	G
1	1A	372	G
1	1A	386	G
1	1A	405	U
1	1A	411	G
1	1A	412	A
1	1A	416	C
1	1A	418	G
1	1A	428	A
1	1A	444	C
1	1A	448	U
1	1A	451	C
1	1A	455	C
1	1A	457	A
1	1A	481	G
1	1A	504	U
1	1A	505	A
1	1A	509	C
1	1A	512	G
1	1A	530	G
1	1A	531	C
1	1A	532	A
1	1A	533	G
1	1A	545	G
1	1A	549	G
1	1A	563	G
1	1A	573	G
1	1A	574	C
1	1A	575	A
1	1A	595	C
1	1A	603	A
1	1A	604	G
1	1A	607	U
1	1A	614	U
1	1A	614(A)	U
1	1A	614(B)	G
1	1A	614(C)	A
1	1A	615	G

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Mol	Chain	Res	Type
1	1A	627	A
1	1A	637	A
1	1A	645	C
1	1A	646	A
1	1A	648	G
1	1A	652(F)	G
1	1A	652(T)	C
1	1A	669	G
1	1A	686	G
1	1A	726	G
1	1A	730	C
1	1A	762	U
1	1A	775	G
1	1A	776	G
1	1A	782	A
1	1A	784	A
1	1A	785	G
1	1A	788	A
1	1A	790	C
1	1A	792	G
1	1A	805	G
1	1A	810	U
1	1A	812	C
1	1A	819	A
1	1A	827	U
1	1A	828	U
1	1A	832	G
1	1A	880	G
1	1A	881	G
1	1A	882	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	896	A
1	1A	897	C
1	1A	898	C
1	1A	900	A

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Mol	Chain	Res	Type
1	1A	907	U
1	1A	910	A
1	1A	932	G
1	1A	938	G
1	1A	945	A
1	1A	946	G
1	1A	953	A
1	1A	958	U
1	1A	959	A
1	1A	961	C
1	1A	968	G
1	1A	974	G
1	1A	975	C
1	1A	975(A)	G
1	1A	983	A
1	1A	996	A
1	1A	1008	C
1	1A	1012	U
1	1A	1013	C
1	1A	1022	G
1	1A	1025	G
1	1A	1026	U
1	1A	1027	A
1	1A	1033	U
1	1A	1038	C
1	1A	1042	G
1	1A	1044	G
1	1A	1045	A
1	1A	1046	A
1	1A	1047	G
1	1A	1048	A
1	1A	1054	A
1	1A	1058	G
1	1A	1059	G
1	1A	1063	G
1	1A	1064	C
1	1A	1066	U
1	1A	1068	G
1	1A	1070	A
1	1A	1071	G
1	1A	1073	A
1	1A	1075	C

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Mol	Chain	Res	Type
1	1A	1076	C
1	1A	1078	U
1	1A	1079	C
1	1A	1081	U
1	1A	1088	A
1	1A	1089	G
1	1A	1090	U
1	1A	1094	U
1	1A	1101	U
1	1A	1106	G
1	1A	1107	G
1	1A	1112	G
1	1A	1129	A
1	1A	1130	U
1	1A	1131	G
1	1A	1135	C
1	1A	1136	G
1	1A	1155	A
1	1A	1156	A
1	1A	1164	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	1195	G
1	1A	1210	A
1	1A	1211	U
1	1A	1218	C
1	1A	1229	G
1	1A	1236	G
1	1A	1237	A
1	1A	1244	G
1	1A	1253	A
1	1A	1256	G
1	1A	1268	A
1	1A	1271	G
1	1A	1272	A
1	1A	1273	U
1	1A	1276	A

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Mol	Chain	Res	Type
1	1A	1298	C
1	1A	1300	U
1	1A	1301	A
1	1A	1318	C
1	1A	1345	C
1	1A	1352	U
1	1A	1359	A
1	1A	1360	A
1	1A	1365	A
1	1A	1372	U
1	1A	1380	G
1	1A	1384	A
1	1A	1385	G
1	1A	1386	C
1	1A	1388	G
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	1439	A
1	1A	1445	A
1	1A	1450	G
1	1A	1455	G
1	1A	1459	G
1	1A	1467	C
1	1A	1482	G
1	1A	1493	C
1	1A	1494	A
1	1A	1496	A
1	1A	1508	A
1	1A	1509	C
1	1A	1509(A)	A
1	1A	1523	U
1	1A	1539	G
1	1A	1540	U
1	1A	1541	G
1	1A	1542	A
1	1A	1543	C
1	1A	1545	A
1	1A	1554	A

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Mol	Chain	Res	Type
1	1A	1558	A
1	1A	1559	G
1	1A	1566	A
1	1A	1569	A
1	1A	1578	U
1	1A	1580	A
1	1A	1581	G
1	1A	1584	C
1	1A	1586	A
1	1A	1602	U
1	1A	1608	A
1	1A	1609	A
1	1A	1610	A
1	1A	1613	G
1	1A	1616	A
1	1A	1648	C
1	1A	1654	A
1	1A	1664	A
1	1A	1674	G
1	1A	1696	G
1	1A	1700	A
1	1A	1701	A
1	1A	1706	U
1	1A	1722	A
1	1A	1746	G
1	1A	1758	G
1	1A	1762	A
1	1A	1763	G
1	1A	1764	G
1	1A	1767	C
1	1A	1773	A
1	1A	1780	A
1	1A	1782	C
1	1A	1791	A
1	1A	1800	C
1	1A	1801	G
1	1A	1816	G
1	1A	1817	G
1	1A	1829	A
1	1A	1847	A
1	1A	1858	G
1	1A	1877	A

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Mol	Chain	Res	Type
1	1A	1878	G
1	1A	1889	A
1	1A	1900	A
1	1A	1906	G
1	1A	1913	A
1	1A	1914	C
1	1A	1915	5MU
1	1A	1929	G
1	1A	1930	G
1	1A	1934	C
1	1A	1936	A
1	1A	1937	A
1	1A	1938	A
1	1A	1952	A
1	1A	1955	U
1	1A	1963	U
1	1A	1964	G
1	1A	1965	C
1	1A	1967	C
1	1A	1970	A
1	1A	1971	A
1	1A	1972	A
1	1A	1984	G
1	1A	1993	U
1	1A	1997	G
1	1A	2001	A
1	1A	2020	A
1	1A	2023	G
1	1A	2027	G
1	1A	2031	A
1	1A	2033	A
1	1A	2035	G
1	1A	2039	C
1	1A	2043	C
1	1A	2049	G
1	1A	2054	A
1	1A	2055	C
1	1A	2056	G
1	1A	2060	A
1	1A	2061	G
1	1A	2062	A
1	1A	2069	G

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Mol	Chain	Res	Type
1	1A	2074	U
1	1A	2078	C
1	1A	2110	G
1	1A	2113	U
1	1A	2114	A
1	1A	2116	G
1	1A	2120	G
1	1A	2122	U
1	1A	2126	A
1	1A	2127	G
1	1A	2129	C
1	1A	2130	U
1	1A	2131	G
1	1A	2132	U
1	1A	2133	G
1	1A	2134	A
1	1A	2135	A
1	1A	2142	C
1	1A	2144	U
1	1A	2146	C
1	1A	2150	U
1	1A	2155	G
1	1A	2157	G
1	1A	2158	A
1	1A	2159	G
1	1A	2162	G
1	1A	2165	G
1	1A	2166	G
1	1A	2171	A
1	1A	2172	U
1	1A	2181	G
1	1A	2182	G
1	1A	2183	C
1	1A	2184	G
1	1A	2189	U
1	1A	2192	G
1	1A	2198	A
1	1A	2206	G
1	1A	2207	G
1	1A	2208	A
1	1A	2219	G
1	1A	2225	A

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Mol	Chain	Res	Type
1	1A	2238	G
1	1A	2239	G
1	1A	2268	A
1	1A	2269	A
1	1A	2279	G
1	1A	2280	G
1	1A	2283	C
1	1A	2287	A
1	1A	2289	G
1	1A	2294	C
1	1A	2305	A
1	1A	2307	G
1	1A	2308	G
1	1A	2314	C
1	1A	2315	G
1	1A	2320	A
1	1A	2325	G
1	1A	2334	G
1	1A	2336	A
1	1A	2347	C
1	1A	2349	G
1	1A	2350	C
1	1A	2361	A
1	1A	2377	A
1	1A	2383	G
1	1A	2385	C
1	1A	2391	G
1	1A	2406	U
1	1A	2410	G
1	1A	2423	U
1	1A	2424	C
1	1A	2425	A
1	1A	2429	G
1	1A	2430	A
1	1A	2435	A
1	1A	2439	A
1	1A	2441	C
1	1A	2447	G
1	1A	2448	A
1	1A	2470	G
1	1A	2476	A
1	1A	2480	C

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Mol	Chain	Res	Type
1	1A	2484	G
1	1A	2490	G
1	1A	2498	C
1	1A	2502	G
1	1A	2504	U
1	1A	2505	G
1	1A	2506	U
1	1A	2518	A
1	1A	2520	C
1	1A	2525	G
1	1A	2529	G
1	1A	2549	G
1	1A	2554	U
1	1A	2555	U
1	1A	2566	A
1	1A	2567	G
1	1A	2579	C
1	1A	2582	G
1	1A	2586	C
1	1A	2588	G
1	1A	2596	U
1	1A	2602	A
1	1A	2609	U
1	1A	2610	C
1	1A	2611	U
1	1A	2612	C
1	1A	2628	C
1	1A	2629	A
1	1A	2630	G
1	1A	2654	A
1	1A	2664	G
1	1A	2689	U
1	1A	2690	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
1	1A	2733	A
1	1A	2757	A
1	1A	2758	A

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Mol	Chain	Res	Type
1	1A	2761	G
1	1A	2764	A
1	1A	2765	A
1	1A	2766	G
1	1A	2769	C
1	1A	2770	G
1	1A	2778	A
1	1A	2780	G
1	1A	2790	A
1	1A	2791	C
1	1A	2792	G
1	1A	2793	G
1	1A	2794	C
1	1A	2802	G
1	1A	2805	G
1	1A	2818	G
1	1A	2820	A
1	1A	2821	A
1	1A	2833	G
1	1A	2835	A
1	1A	2850	A
1	1A	2872	G
1	1A	2873	A
1	1A	2879	C
1	1A	2880	C
1	1A	2889	C
1	1A	2892	A
1	1A	2894	G
2	1B	2	C
2	1B	5	C
2	1B	13	A
2	1B	15	A
2	1B	42	C
2	1B	44	G
2	1B	45	A
2	1B	53	A
2	1B	56	G
2	1B	63	G
2	1B	73	A
2	1B	85	G
2	1B	106	G
2	1B	110	G

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Mol	Chain	Res	Type
32	1a	9	G
32	1a	31	G
32	1a	32	A
32	1a	39	G
32	1a	44	G
32	1a	47	C
32	1a	48	C
32	1a	51	A
32	1a	61	G
32	1a	73	G
32	1a	79	G
32	1a	91	C
32	1a	97	G
32	1a	98	G
32	1a	101	A
32	1a	105	G
32	1a	111	G
32	1a	116	A
32	1a	121	C
32	1a	131	C
32	1a	159	G
32	1a	163	C
32	1a	174	C
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	199	G
32	1a	201	C
32	1a	202	U
32	1a	203	U
32	1a	204	U
32	1a	222	U
32	1a	245	C
32	1a	247	G
32	1a	251	G
32	1a	258	G
32	1a	266	G
32	1a	267	C
32	1a	279	A

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Mol	Chain	Res	Type
32	1a	289	G
32	1a	306	G
32	1a	313	A
32	1a	321	A
32	1a	328	C
32	1a	332	G
32	1a	348	G
32	1a	351	G
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	363	A
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	375	U
32	1a	381	C
32	1a	388	G
32	1a	390	C
32	1a	397	A
32	1a	398	C
32	1a	406	G
32	1a	412	A
32	1a	413	G
32	1a	421	U
32	1a	423	G
32	1a	424	G
32	1a	429	U
32	1a	430	A
32	1a	431	A
32	1a	439	A
32	1a	441	A
32	1a	442	C
32	1a	452	A
32	1a	461	A
32	1a	470	C
32	1a	476	G
32	1a	485	G
32	1a	492	G
32	1a	496	A
32	1a	498	U
32	1a	505	G

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Mol	Chain	Res	Type
32	1a	509	A
32	1a	510	A
32	1a	511	C
32	1a	518	C
32	1a	519	C
32	1a	524	G
32	1a	527	7MG
32	1a	531	U
32	1a	532	A
32	1a	533	A
32	1a	536	C
32	1a	547	A
32	1a	559	A
32	1a	561	U
32	1a	562	C
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	577	G
32	1a	596	C
32	1a	630	G
32	1a	653	A
32	1a	665	A
32	1a	671	G
32	1a	687	A
32	1a	688	G
32	1a	702	A
32	1a	721	G
32	1a	723	U
32	1a	724	G
32	1a	731	G
32	1a	749	C
32	1a	755	G
32	1a	763	G
32	1a	766	A
32	1a	777	A
32	1a	792	A
32	1a	793	U
32	1a	794	A
32	1a	802	A
32	1a	810	C
32	1a	812	C

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Mol	Chain	Res	Type
32	1a	817	C
32	1a	821	G
32	1a	827	U
32	1a	828	A
32	1a	833	U
32	1a	834	C
32	1a	840	C
32	1a	841	U
32	1a	851	G
32	1a	853	G
32	1a	859	A
32	1a	864	A
32	1a	870	U
32	1a	872	A
32	1a	876	G
32	1a	885	G
32	1a	889	A
32	1a	902	G
32	1a	914	A
32	1a	916	G
32	1a	926	G
32	1a	927	G
32	1a	934	C
32	1a	935	A
32	1a	942	G
32	1a	944	G
32	1a	958	A
32	1a	960	U
32	1a	961	U
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	972	C
32	1a	974	A
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	982	U
32	1a	992	U
32	1a	993	G
32	1a	994	A
32	1a	997	U

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Mol	Chain	Res	Type
32	1a	1000	U
32	1a	1002	G
32	1a	1003	G
32	1a	1005	A
32	1a	1006	C
32	1a	1020	U
32	1a	1022	G
32	1a	1026	G
32	1a	1027	C
32	1a	1030	C
32	1a	1030(A)	G
32	1a	1030(C)	G
32	1a	1031	G
32	1a	1033	G
32	1a	1037	C
32	1a	1044	A
32	1a	1046	A
32	1a	1053	G
32	1a	1054	C
32	1a	1063	C
32	1a	1066	C
32	1a	1068	G
32	1a	1081	G
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1103	C
32	1a	1108	G
32	1a	1121	U
32	1a	1122	U
32	1a	1124	G
32	1a	1125	U
32	1a	1134	G
32	1a	1136	U
32	1a	1137	C
32	1a	1138	G
32	1a	1139	G
32	1a	1141	C
32	1a	1146	A
32	1a	1151	A
32	1a	1152	A
32	1a	1157	A

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Mol	Chain	Res	Type
32	1a	1159	U
32	1a	1166	G
32	1a	1184	G
32	1a	1189	C
32	1a	1193	G
32	1a	1196	U
32	1a	1201	A
32	1a	1202	G
32	1a	1212	U
32	1a	1213	A
32	1a	1214	C
32	1a	1227	A
32	1a	1236	A
32	1a	1238	A
32	1a	1256	A
32	1a	1257	U
32	1a	1258	G
32	1a	1270	C
32	1a	1275	A
32	1a	1276	G
32	1a	1278	U
32	1a	1279	A
32	1a	1280	A
32	1a	1286	A
32	1a	1287	A
32	1a	1293	G
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1305	G
32	1a	1317	C
32	1a	1319	A
32	1a	1320	C
32	1a	1322	C
32	1a	1323	G
32	1a	1334	G
32	1a	1338	G
32	1a	1340	A
32	1a	1346	A
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C

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Mol	Chain	Res	Type
32	1a	1363(A)	A
32	1a	1370	G
32	1a	1381	U
32	1a	1384	C
32	1a	1390	U
32	1a	1399	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	1456	G
32	1a	1487	G
32	1a	1492	A
32	1a	1494	G
32	1a	1497	G
32	1a	1503	A
32	1a	1504	G
32	1a	1506	U
32	1a	1517	G
32	1a	1520	G
32	1a	1529	G
32	1a	1530	G
32	1a	1532	U
53	1v	13	A
53	1v	14	A
53	1v	15	A
53	1v	19	U
53	1v	23	A
53	1v	24	A
54	1x	6	G
54	1x	9	G
54	1x	14	A
54	1x	17(A)	U
54	1x	18	G
54	1x	19	G
54	1x	21	A
54	1x	31	G
54	1x	32	5MC
54	1x	47	U
54	1x	69	C

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Mol	Chain	Res	Type
1	2A	12	U
1	2A	14	A
1	2A	15	G
1	2A	32	C
1	2A	34	C
1	2A	35	G
1	2A	45	C
1	2A	50	U
1	2A	63	U
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	99	U
1	2A	100	G
1	2A	102	G
1	2A	112	U
1	2A	118	A
1	2A	120	U
1	2A	128	C
1	2A	154(A)	C
1	2A	157	U
1	2A	181	A
1	2A	196	A
1	2A	199	A
1	2A	204	A
1	2A	205	G
1	2A	214	G
1	2A	216	A
1	2A	221	A
1	2A	222	A
1	2A	227	A
1	2A	228	A
1	2A	229	A
1	2A	232	G
1	2A	248	G
1	2A	249	C
1	2A	250	G
1	2A	266	G
1	2A	267	C

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Mol	Chain	Res	Type
1	2A	271(K)	U
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	271(O)	C
1	2A	271(T)	C
1	2A	272	G
1	2A	272(B)	G
1	2A	277	C
1	2A	278	A
1	2A	279	C
1	2A	283	A
1	2A	294	A
1	2A	311	A
1	2A	316	C
1	2A	324	A
1	2A	327	G
1	2A	329	G
1	2A	330	A
1	2A	342	G
1	2A	346	A
1	2A	352	G
1	2A	354	G
1	2A	362	U
1	2A	363	G
1	2A	363(B)	G
1	2A	366	C
1	2A	370	G
1	2A	386	G
1	2A	396	G
1	2A	399	G
1	2A	405	U
1	2A	407	G
1	2A	411	G
1	2A	412	A
1	2A	422	A
1	2A	427	U
1	2A	435	C
1	2A	444	C
1	2A	454	A
1	2A	456	C
1	2A	457	A

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Mol	Chain	Res	Type
1	2A	459	U
1	2A	481	G
1	2A	504	U
1	2A	505	A
1	2A	508	G
1	2A	509	C
1	2A	527	C
1	2A	528	A
1	2A	529	A
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	533	G
1	2A	545	G
1	2A	551	G
1	2A	556	G
1	2A	563	G
1	2A	573	G
1	2A	574	C
1	2A	575	A
1	2A	586	A
1	2A	588	U
1	2A	595	C
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	614(A)	U
1	2A	614(B)	G
1	2A	615	G
1	2A	616	G
1	2A	620	G
1	2A	627	A
1	2A	637	A
1	2A	645	C
1	2A	649	G
1	2A	652(B)	A
1	2A	652(C)	G
1	2A	669	G
1	2A	686	G
1	2A	698	C
1	2A	699	A
1	2A	730	C

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Mol	Chain	Res	Type
1	2A	738	G
1	2A	753	C
1	2A	764	A
1	2A	771	G
1	2A	775	G
1	2A	776	G
1	2A	778	G
1	2A	779	U
1	2A	782	A
1	2A	784	A
1	2A	785	G
1	2A	792	G
1	2A	794	G
1	2A	805	G
1	2A	812	C
1	2A	819	A
1	2A	827	U
1	2A	828	U
1	2A	846	C
1	2A	847	U
1	2A	857	C
1	2A	859	G
1	2A	866	A
1	2A	869	G
1	2A	870	A
1	2A	874	G
1	2A	878	A
1	2A	879	G
1	2A	880	G
1	2A	884	C
1	2A	886	C
1	2A	887	A
1	2A	888	C
1	2A	889	C
1	2A	892	G
1	2A	893	C
1	2A	894	C
1	2A	896	A
1	2A	897	C
1	2A	900	A
1	2A	901	A
1	2A	904	C

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Mol	Chain	Res	Type
1	2A	910	A
1	2A	914	C
1	2A	917	A
1	2A	926	A
1	2A	932	G
1	2A	933	A
1	2A	936	C
1	2A	941	A
1	2A	945	A
1	2A	946	G
1	2A	953	A
1	2A	958	U
1	2A	959	A
1	2A	961	C
1	2A	974	G
1	2A	975	C
1	2A	983	A
1	2A	996	A
1	2A	997	G
1	2A	998	C
1	2A	1012	U
1	2A	1013	C
1	2A	1017	G
1	2A	1021	A
1	2A	1022	G
1	2A	1023	U
1	2A	1025	G
1	2A	1026	U
1	2A	1033	U
1	2A	1038	C
1	2A	1039	G
1	2A	1043	C
1	2A	1114	G
1	2A	1116	C
1	2A	1122	G
1	2A	1131	G
1	2A	1135	C
1	2A	1136	G
1	2A	1139	G
1	2A	1142	U
1	2A	1142(A)	A
1	2A	1144	G

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Mol	Chain	Res	Type
1	2A	1155	A
1	2A	1169	G
1	2A	1170	G
1	2A	1171	G
1	2A	1195	G
1	2A	1204	A
1	2A	1210	A
1	2A	1211	U
1	2A	1218	C
1	2A	1220	A
1	2A	1224	C
1	2A	1229	G
1	2A	1237	A
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A
1	2A	1273	U
1	2A	1289	C
1	2A	1298	C
1	2A	1300	U
1	2A	1301	A
1	2A	1314	C
1	2A	1318	C
1	2A	1321	A
1	2A	1327	C
1	2A	1345	C
1	2A	1352	U
1	2A	1359	A
1	2A	1360	A
1	2A	1365	A
1	2A	1368	G
1	2A	1370	C
1	2A	1378	A
1	2A	1380	G
1	2A	1383	C
1	2A	1384	A
1	2A	1385	G
1	2A	1386	C
1	2A	1400	G
1	2A	1412	A
1	2A	1416	G

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Mol	Chain	Res	Type
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	1441	G
1	2A	1445	A
1	2A	1445(A)	C
1	2A	1449	A
1	2A	1450	G
1	2A	1455	G
1	2A	1460	A
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	1496	A
1	2A	1497	U
1	2A	1506	C
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1525	G
1	2A	1531	C
1	2A	1538	G
1	2A	1541	G
1	2A	1543	C
1	2A	1544	A
1	2A	1545	A
1	2A	1558	A
1	2A	1559	G
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1580	A
1	2A	1584	C
1	2A	1586	A
1	2A	1587	A
1	2A	1594	G

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Mol	Chain	Res	Type
1	2A	1602	U
1	2A	1603	A
1	2A	1608	A
1	2A	1609	A
1	2A	1610	A
1	2A	1640	C
1	2A	1646	C
1	2A	1647	G
1	2A	1648	C
1	2A	1649	G
1	2A	1654	A
1	2A	1663	C
1	2A	1674	G
1	2A	1675	C
1	2A	1696	G
1	2A	1700	A
1	2A	1701	A
1	2A	1722	A
1	2A	1739	U
1	2A	1745(A)	C
1	2A	1746	G
1	2A	1756	G
1	2A	1758	G
1	2A	1762	A
1	2A	1763	G
1	2A	1764	G
1	2A	1769	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	1816	G
1	2A	1835	G
1	2A	1847	A
1	2A	1848	A
1	2A	1877	A
1	2A	1878	G
1	2A	1900	A
1	2A	1906	G
1	2A	1913	A

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Mol	Chain	Res	Type
1	2A	1914	C
1	2A	1929	G
1	2A	1930	G
1	2A	1931	U
1	2A	1936	A
1	2A	1937	A
1	2A	1938	A
1	2A	1955	U
1	2A	1963	U
1	2A	1964	G
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1993	U
1	2A	1994	C
1	2A	1996	C
1	2A	1997	G
1	2A	2020	A
1	2A	2023	G
1	2A	2031	A
1	2A	2033	A
1	2A	2043	C
1	2A	2055	C
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G
1	2A	2062	A
1	2A	2069	G
1	2A	2096	U
1	2A	2099	U
1	2A	2105	C
1	2A	2108	C
1	2A	2111	C
1	2A	2112	G
1	2A	2116	G
1	2A	2119	A
1	2A	2120	G
1	2A	2122	U
1	2A	2124	G
1	2A	2125	G
1	2A	2126	A

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Mol	Chain	Res	Type
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	2137	C
1	2A	2138	C
1	2A	2140	C
1	2A	2142	C
1	2A	2143	C
1	2A	2144	U
1	2A	2146	C
1	2A	2147	G
1	2A	2148	G
1	2A	2150	U
1	2A	2154	G
1	2A	2155	G
1	2A	2156	G
1	2A	2157	G
1	2A	2158	A
1	2A	2161	C
1	2A	2162	G
1	2A	2164	C
1	2A	2165	G
1	2A	2166	G
1	2A	2167	U
1	2A	2172	U
1	2A	2174	C
1	2A	2185	C
1	2A	2189	U
1	2A	2192	G
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2218	U
1	2A	2225	A
1	2A	2234	G
1	2A	2235	G
1	2A	2238	G

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Mol	Chain	Res	Type
1	2A	2239	G
1	2A	2268	A
1	2A	2275	C
1	2A	2279	G
1	2A	2283	C
1	2A	2287	A
1	2A	2288	A
1	2A	2289	G
1	2A	2300	G
1	2A	2302	G
1	2A	2305	A
1	2A	2307	G
1	2A	2308	G
1	2A	2315	G
1	2A	2320	A
1	2A	2325	G
1	2A	2327	A
1	2A	2334	G
1	2A	2336	A
1	2A	2347	C
1	2A	2350	C
1	2A	2352	A
1	2A	2353	G
1	2A	2366	A
1	2A	2372	G
1	2A	2376	A
1	2A	2383	G
1	2A	2385	C
1	2A	2391	G
1	2A	2406	U
1	2A	2422	A
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	2474	C
1	2A	2476	A
1	2A	2482	G

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Mol	Chain	Res	Type
1	2A	2502	G
1	2A	2505	G
1	2A	2506	U
1	2A	2507	C
1	2A	2518	A
1	2A	2520	C
1	2A	2525	G
1	2A	2529	G
1	2A	2554	U
1	2A	2555	U
1	2A	2556	C
1	2A	2566	A
1	2A	2567	G
1	2A	2574	G
1	2A	2577	A
1	2A	2579	C
1	2A	2582	G
1	2A	2586	C
1	2A	2602	A
1	2A	2611	U
1	2A	2612	C
1	2A	2630	G
1	2A	2634	G
1	2A	2654	A
1	2A	2666	C
1	2A	2684	U
1	2A	2689	U
1	2A	2690	C
1	2A	2691	C
1	2A	2702	U
1	2A	2703	C
1	2A	2707	G
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G
1	2A	2726	U
1	2A	2733	A
1	2A	2744	G
1	2A	2751	G
1	2A	2758	A
1	2A	2761	G
1	2A	2764	A

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Mol	Chain	Res	Type
1	2A	2765	A
1	2A	2766	G
1	2A	2778	A
1	2A	2789	C
1	2A	2793	G
1	2A	2802	G
1	2A	2804	C
1	2A	2807	G
1	2A	2810	A
1	2A	2820	A
1	2A	2821	A
1	2A	2823	A
1	2A	2830	G
1	2A	2833	G
1	2A	2834	G
1	2A	2835	A
1	2A	2872	G
1	2A	2880	C
1	2A	2892	A
1	2A	2894	G
1	2A	2896	C
1	2A	2897	U
2	2B	2	C
2	2B	5	C
2	2B	8	U
2	2B	13	A
2	2B	16	G
2	2B	19	G
2	2B	20	C
2	2B	24	G
2	2B	25	A
2	2B	30	C
2	2B	32	C
2	2B	42	C
2	2B	52	A
2	2B	53	A
2	2B	56	G
2	2B	58	A
2	2B	63	G
2	2B	64	C
2	2B	65	C
2	2B	66	A

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Mol	Chain	Res	Type
2	2B	67	G
2	2B	72	G
2	2B	73	A
2	2B	74	U
2	2B	85	G
2	2B	106	G
2	2B	108	U
2	2B	110	G
2	2B	114	C
2	2B	116	G
2	2B	120	A
32	2a	6	G
32	2a	9	G
32	2a	15	G
32	2a	21	G
32	2a	22	G
32	2a	26	A
32	2a	32	A
32	2a	39	G
32	2a	48	C
32	2a	51	A
32	2a	54	C
32	2a	65	U
32	2a	66	G
32	2a	73	G
32	2a	80	G
32	2a	88	A
32	2a	89	C
32	2a	98	G
32	2a	101	A
32	2a	116	A
32	2a	120	A
32	2a	121	C
32	2a	131	C
32	2a	144	G
32	2a	159	G
32	2a	163	C
32	2a	174	C
32	2a	182	U
32	2a	189(E)	U
32	2a	189(F)	U
32	2a	189(K)	U

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Mol	Chain	Res	Type
32	2a	195	A
32	2a	197	A
32	2a	202	U
32	2a	203	U
32	2a	204	U
32	2a	216	G
32	2a	247	G
32	2a	251	G
32	2a	258	G
32	2a	266	G
32	2a	267	C
32	2a	269	C
32	2a	289	G
32	2a	306	G
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	350	G
32	2a	352	C
32	2a	353	A
32	2a	354	G
32	2a	367	U
32	2a	372	C
32	2a	373	A
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	412	A
32	2a	422	C
32	2a	423	G
32	2a	424	G
32	2a	429	U
32	2a	430	A
32	2a	439	A
32	2a	441	A
32	2a	442	C
32	2a	452	A
32	2a	461	A
32	2a	470	C
32	2a	471	G
32	2a	485	G
32	2a	496	A

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Mol	Chain	Res	Type
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	531	U
32	2a	532	A
32	2a	533	A
32	2a	547	A
32	2a	559	A
32	2a	564	C
32	2a	568	G
32	2a	572	A
32	2a	573	A
32	2a	576	G
32	2a	577	G
32	2a	588	G
32	2a	596	C
32	2a	607	A
32	2a	618	C
32	2a	630	G
32	2a	631	G
32	2a	653	A
32	2a	665	A
32	2a	681	C
32	2a	687	A
32	2a	688	G
32	2a	702	A
32	2a	712	A
32	2a	723	U
32	2a	724	G
32	2a	731	G
32	2a	733	A
32	2a	734	G
32	2a	749	C
32	2a	755	G
32	2a	760	G
32	2a	763	G
32	2a	777	A

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Mol	Chain	Res	Type
32	2a	793	U
32	2a	794	A
32	2a	815	A
32	2a	816	A
32	2a	817	C
32	2a	821	G
32	2a	828	A
32	2a	840	C
32	2a	841	U
32	2a	855	G
32	2a	859	A
32	2a	873	A
32	2a	902	G
32	2a	914	A
32	2a	922	G
32	2a	926	G
32	2a	927	G
32	2a	931	C
32	2a	934	C
32	2a	935	A
32	2a	941	G
32	2a	953	G
32	2a	960	U
32	2a	961	U
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	992	U
32	2a	993	G
32	2a	997	U
32	2a	998	G
32	2a	1000	U
32	2a	1001(A)	G
32	2a	1002	G
32	2a	1003	G
32	2a	1005	A
32	2a	1006	C

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Mol	Chain	Res	Type
32	2a	1009	G
32	2a	1011	G
32	2a	1020	U
32	2a	1021	G
32	2a	1022	G
32	2a	1025	U
32	2a	1026	G
32	2a	1027	C
32	2a	1030(A)	G
32	2a	1031	G
32	2a	1038	C
32	2a	1039	C
32	2a	1040	U
32	2a	1045	C
32	2a	1048	G
32	2a	1051	C
32	2a	1053	G
32	2a	1054	C
32	2a	1055	A
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1077	G
32	2a	1081	G
32	2a	1086	U
32	2a	1094	G
32	2a	1095	U
32	2a	1101	A
32	2a	1104	G
32	2a	1113	C
32	2a	1114	C
32	2a	1117	G
32	2a	1122	U
32	2a	1125	U
32	2a	1129	C
32	2a	1130	A
32	2a	1136	U
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G
32	2a	1140	C
32	2a	1141	C

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Mol	Chain	Res	Type
32	2a	1146	A
32	2a	1147	C
32	2a	1151	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	1211	U
32	2a	1212	U
32	2a	1213	A
32	2a	1220	G
32	2a	1227	A
32	2a	1238	A
32	2a	1240	U
32	2a	1241	G
32	2a	1248	A
32	2a	1255	G
32	2a	1256	A
32	2a	1257	U
32	2a	1260	C
32	2a	1261	A
32	2a	1262	C
32	2a	1263	C
32	2a	1270	C
32	2a	1272	G
32	2a	1275	A
32	2a	1277	C
32	2a	1278	U
32	2a	1279	A
32	2a	1280	A
32	2a	1283	G
32	2a	1287	A
32	2a	1294	G
32	2a	1303	C
32	2a	1320	C
32	2a	1322	C

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Mol	Chain	Res	Type
32	2a	1323	G
32	2a	1324	A
32	2a	1346	A
32	2a	1347	G
32	2a	1358	U
32	2a	1363	C
32	2a	1364	U
32	2a	1370	G
32	2a	1397	C
32	2a	1400	5MC
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1447	A
32	2a	1452	C
32	2a	1456	G
32	2a	1457	G
32	2a	1487	G
32	2a	1492	A
32	2a	1494	G
32	2a	1497	G
32	2a	1503	A
32	2a	1504	G
32	2a	1506	U
32	2a	1507	A
32	2a	1517	G
32	2a	1520	G
32	2a	1529	G
32	2a	1530	G
53	2v	13	A
53	2v	14	A
53	2v	15	A
53	2v	19	U
54	2x	9	G
54	2x	13	C
54	2x	21	A
54	2x	22	G
54	2x	25	C
54	2x	46	G
54	2x	47	U
54	2x	48	C
54	2x	52	G

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Mol	Chain	Res	Type
54	2x	56	C
54	2x	63	G
54	2x	68	C
54	2x	76	A

All (51) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	90	U
1	1A	196	A
1	1A	266	G
1	1A	278	A
1	1A	351	G
1	1A	548	A
1	1A	895	U
1	1A	1047	G
1	1A	1065	U
1	1A	1067	A
1	1A	1142(A)	A
1	1A	1174	A
1	1A	1176	G
1	1A	1210	A
1	1A	1275	A
1	1A	1379	A
1	1A	1442	G
1	1A	1508	A
1	1A	1608	A
1	1A	1653	G
1	1A	1992	G
1	1A	2126	A
1	1A	2134	A
1	1A	2181	G
1	1A	2183	C
1	1A	2430	A
1	1A	2629	A
1	1A	2689	U
1	1A	2756	U
2	1B	1	U
1	2A	228	A
1	2A	266	G
1	2A	271(M)	G
1	2A	277	C

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Mol	Chain	Res	Type
1	2A	528	A
1	2A	752	A
1	2A	805	G
1	2A	856	C
1	2A	900	A
1	2A	1210	A
1	2A	1379	A
1	2A	1420	U
1	2A	1442	G
1	2A	1530	C
1	2A	1653	G
1	2A	1913	A
1	2A	1992	G
1	2A	2119	A
1	2A	2126	A
1	2A	2351	G
1	2A	2689	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	PSU	2A	1917	1	18,21,22	1.36	2 (11%)	22,30,33	1.94	3 (13%)
54	PSU	2x	55	54	18,21,22	1.34	2 (11%)	22,30,33	1.79	4 (18%)
1	4OC	1A	1920	1	19,22,24	0.86	0	26,31,35	0.96	1 (3%)
1	2MA	1A	2503	56,1	17,25,26	0.96	0	17,37,40	0.97	2 (11%)
32	5MC	2a	1404	32	18,22,23	0.92	2 (11%)	26,32,35	1.08	2 (7%)
1	5MU	2A	1939	1	19,22,23	1.50	5 (26%)	28,32,35	2.31	8 (28%)
1	5MU	1A	1939	1	19,22,23	1.46	5 (26%)	28,32,35	2.03	5 (17%)
32	5MC	1a	967	32	18,22,23	0.98	2 (11%)	26,32,35	1.06	3 (11%)
32	M2G	2a	966	32	20,27,28	1.55	3 (15%)	22,40,43	0.85	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	2MU	2A	2552	56,1	19,22,24	1.27	3 (15%)	26,31,36	1.82	6 (23%)
32	5MC	2a	1400	32	18,22,23	0.98	2 (11%)	26,32,35	1.17	3 (11%)
43	0TD	2l	92	43	7,9,10	4.72	1 (14%)	6,11,13	9.41	1 (16%)
32	MA6	1a	1518	32	19,26,27	0.98	1 (5%)	18,38,41	1.69	5 (27%)
54	5MU	1x	54	54	19,22,23	1.39	5 (26%)	28,32,35	1.88	6 (21%)
32	7MG	1a	527	56,32	22,26,27	1.40	4 (18%)	29,39,42	2.44	7 (24%)
1	5MU	1A	1915	1	19,22,23	1.46	4 (21%)	28,32,35	2.09	7 (25%)
32	5MC	1a	1400	32	18,22,23	1.00	2 (11%)	26,32,35	1.20	4 (15%)
32	MA6	2a	1519	32	19,26,27	0.95	1 (5%)	18,38,41	1.58	4 (22%)
1	PSU	1A	1917	1	18,21,22	1.34	2 (11%)	22,30,33	1.83	3 (13%)
1	PSU	1A	2605	1	18,21,22	1.37	3 (16%)	22,30,33	1.73	4 (18%)
1	5MC	2A	1942	1	18,22,23	0.98	2 (11%)	26,32,35	1.19	2 (7%)
32	2MG	1a	1207	32	18,26,27	0.97	1 (5%)	16,38,41	1.27	3 (18%)
1	5MC	1A	1942	56,1	18,22,23	0.98	2 (11%)	26,32,35	1.09	2 (7%)
1	2MA	2A	2503	56,1	17,25,26	1.02	1 (5%)	17,37,40	0.96	2 (11%)
54	5MC	1x	32	54	18,22,23	1.06	2 (11%)	26,32,35	1.38	4 (15%)
32	UR3	2a	1498	32	19,22,23	0.95	0	26,32,35	1.50	2 (7%)
32	MA6	1a	1519	32	19,26,27	1.02	1 (5%)	18,38,41	1.69	5 (27%)
1	PSU	2A	1911	1	18,21,22	1.35	3 (16%)	22,30,33	1.83	3 (13%)
32	4OC	1a	1402	32	20,23,24	0.73	0	26,32,35	0.90	1 (3%)
54	4SU	1x	8	54	18,21,22	1.99	4 (22%)	26,30,33	1.52	2 (7%)
1	4OC	2A	1920	1	19,22,24	0.79	0	26,31,35	1.08	2 (7%)
32	MA6	2a	1518	32	19,26,27	0.98	1 (5%)	18,38,41	1.72	5 (27%)
32	M2G	1a	966	32	20,27,28	1.35	3 (15%)	22,40,43	0.98	2 (9%)
1	5MC	2A	1962	56,1	18,22,23	0.99	2 (11%)	26,32,35	1.25	3 (11%)
32	7MG	2a	527	32	22,26,27	1.37	4 (18%)	29,39,42	2.44	7 (24%)
32	UR3	1a	1498	32	19,22,23	1.02	1 (5%)	26,32,35	1.50	2 (7%)
1	5MC	1A	1962	56,1	18,22,23	0.95	2 (11%)	26,32,35	1.10	2 (7%)
32	PSU	1a	516	56,32	18,21,22	1.37	2 (11%)	22,30,33	1.82	3 (13%)
32	5MC	1a	1404	32	18,22,23	1.00	2 (11%)	26,32,35	1.21	5 (19%)
1	5MU	2A	1915	56,1	19,22,23	1.44	6 (31%)	28,32,35	2.07	7 (25%)
32	5MC	2a	1407	32	18,22,23	0.98	2 (11%)	26,32,35	1.13	3 (11%)
1	OMG	1A	2251	56,1,54	18,26,27	1.08	1 (5%)	19,38,41	1.03	2 (10%)
54	4SU	2x	8	54	18,21,22	1.95	6 (33%)	26,30,33	1.60	6 (23%)
54	5MC	2x	32	54	18,22,23	0.93	2 (11%)	26,32,35	1.15	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
54	5MU	2x	54	54	19,22,23	1.44	4 (21%)	28,32,35	1.98	6 (21%)
1	PSU	1A	1911	1	18,21,22	1.37	3 (16%)	22,30,33	1.85	3 (13%)
1	2MU	1A	2552	56,1	19,22,24	1.19	2 (10%)	26,31,36	1.92	6 (23%)
32	2MG	2a	1207	32	18,26,27	0.90	0	16,38,41	1.02	2 (12%)
1	PSU	2A	2605	1	18,21,22	1.38	3 (16%)	22,30,33	1.85	3 (13%)
1	OMG	2A	2251	56,1,54	18,26,27	0.91	1 (5%)	19,38,41	1.10	2 (10%)
32	5MC	1a	1407	32	18,22,23	0.94	1 (5%)	26,32,35	1.11	2 (7%)
54	PSU	1x	55	56,54	18,21,22	1.30	2 (11%)	22,30,33	1.93	4 (18%)
32	PSU	2a	516	32	18,21,22	1.35	2 (11%)	22,30,33	1.83	4 (18%)
32	5MC	2a	967	32	18,22,23	1.00	1 (5%)	26,32,35	1.10	3 (11%)
32	4OC	2a	1402	56,32	20,23,24	0.78	0	26,32,35	0.98	1 (3%)
43	0TD	1l	92	43	7,9,10	4.70	1 (14%)	6,11,13	3.41	2 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
54	PSU	2x	55	54	-	0/7/25/26	0/2/2/2
1	4OC	1A	1920	1	-	0/9/27/30	0/2/2/2
1	2MA	1A	2503	56,1	-	2/3/25/26	0/3/3/3
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	1	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	1/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	4/7/29/30	0/3/3/3
1	2MU	2A	2552	56,1	-	1/9/27/28	0/2/2/2
32	5MC	2a	1400	32	-	2/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	3/7/12/14	-
32	MA6	1a	1518	32	-	3/7/29/30	0/3/3/3
54	5MU	1x	54	54	-	0/7/25/26	0/2/2/2
32	7MG	1a	527	56,32	-	2/7/37/38	0/3/3/3
1	5MU	1A	1915	1	-	2/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	5/7/29/30	0/3/3/3
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	1A	2605	1	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	0/5/27/28	0/3/3/3
1	5MC	1A	1942	56,1	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	56,1	-	1/3/25/26	0/3/3/3
54	5MC	1x	32	54	-	0/7/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	4/7/29/30	0/3/3/3
1	PSU	2A	1911	1	-	1/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	4/9/29/30	0/2/2/2
54	4SU	1x	8	54	-	0/7/25/26	0/2/2/2
1	4OC	2A	1920	1	-	2/9/27/30	0/2/2/2
32	MA6	2a	1518	32	-	3/7/29/30	0/3/3/3
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
1	5MC	2A	1962	56,1	-	2/7/25/26	0/2/2/2
32	7MG	2a	527	32	-	2/7/37/38	0/3/3/3
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
1	5MC	1A	1962	56,1	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	56,32	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	56,1	-	0/7/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
1	OMG	1A	2251	56,1,54	-	0/5/27/28	0/3/3/3
54	4SU	2x	8	54	-	0/7/25/26	0/2/2/2
54	5MC	2x	32	54	-	0/7/25/26	0/2/2/2
54	5MU	2x	54	54	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
1	2MU	1A	2552	56,1	-	0/9/27/28	0/2/2/2
32	2MG	2a	1207	32	-	0/5/27/28	0/3/3/3
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	56,1,54	-	1/5/27/28	0/3/3/3
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
54	PSU	1x	55	56,54	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	56,32	-	4/9/29/30	0/2/2/2
43	0TD	1l	92	43	-	3/7/12/14	-

All (119) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.21	1.69	1.82
43	1l	92	0TD	CB-SB	-11.99	1.70	1.82
32	2a	966	M2G	C2-N3	5.01	1.36	1.30
54	1x	8	4SU	C4-S4	-4.53	1.59	1.68
54	2x	8	4SU	C4-S4	-4.16	1.60	1.68
54	2x	8	4SU	C4-N3	-4.15	1.33	1.37
54	1x	8	4SU	C4-N3	-4.14	1.33	1.37
32	1a	966	M2G	C2-N3	4.05	1.35	1.30
54	1x	8	4SU	C2-N3	-3.67	1.31	1.38
1	2A	1917	PSU	C6-C5	3.51	1.39	1.35
54	2x	55	PSU	C6-C5	3.46	1.39	1.35
32	2a	516	PSU	C6-C5	3.38	1.39	1.35
54	1x	32	5MC	C6-C5	3.31	1.40	1.34
1	1A	1917	PSU	C6-C5	3.31	1.39	1.35
1	1A	1911	PSU	C6-C5	3.28	1.39	1.35
54	2x	8	4SU	C5-C4	-3.25	1.38	1.42
32	1a	516	PSU	C6-C5	3.24	1.39	1.35
54	1x	55	PSU	C6-C5	3.20	1.39	1.35
54	1x	8	4SU	C5-C4	-3.20	1.38	1.42
32	1a	527	7MG	C4-N9	-3.15	1.34	1.37
1	2A	1911	PSU	C6-C5	3.12	1.39	1.35
32	1a	527	7MG	C5-C4	3.10	1.48	1.38
1	2A	2605	PSU	C6-C5	3.04	1.38	1.35
32	2a	527	7MG	C4-N9	-3.04	1.34	1.37
54	2x	54	5MU	C6-C5	3.03	1.39	1.34
32	2a	967	5MC	C6-C5	3.03	1.39	1.34
32	2a	527	7MG	C5-C4	2.99	1.47	1.38
1	1A	2605	PSU	C6-C5	2.98	1.38	1.35
1	1A	2251	OMG	C6-N1	-2.95	1.33	1.37
32	1a	1400	5MC	C6-C5	2.93	1.39	1.34
1	2A	2605	PSU	C4-N3	-2.92	1.33	1.38
32	2a	966	M2G	C2-N2	2.92	1.40	1.35
1	1A	2552	2MU	C4-N3	-2.91	1.33	1.38
1	1A	1939	5MU	C4-N3	-2.89	1.33	1.38
32	1a	1207	2MG	C6-N1	-2.88	1.33	1.37
54	1x	54	5MU	C4-N3	-2.88	1.33	1.38
1	2A	1939	5MU	C4-N3	-2.86	1.33	1.38
1	2A	1915	5MU	C6-C5	2.85	1.39	1.34
54	1x	54	5MU	C6-C5	2.84	1.39	1.34
1	2A	1939	5MU	C4-C5	2.82	1.49	1.44
32	1a	1407	5MC	C6-C5	2.81	1.39	1.34
1	1A	2605	PSU	C4-N3	-2.79	1.33	1.38
32	1a	966	M2G	C6-N1	-2.79	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1a	967	5MC	C6-C5	2.78	1.39	1.34
1	1A	1915	5MU	C6-C5	2.78	1.39	1.34
1	2A	1939	5MU	C6-C5	2.77	1.39	1.34
1	1A	1939	5MU	C6-C5	2.77	1.39	1.34
32	2a	1400	5MC	C6-C5	2.77	1.39	1.34
1	1A	1915	5MU	C2-N1	2.76	1.42	1.38
1	1A	1942	5MC	C6-C5	2.76	1.39	1.34
1	2A	1962	5MC	C6-C5	2.75	1.39	1.34
1	2A	2552	2MU	C4-N3	-2.74	1.33	1.38
32	2a	1404	5MC	C6-C5	2.69	1.39	1.34
1	1A	1915	5MU	C4-C5	2.68	1.49	1.44
1	2A	1915	5MU	C4-C5	2.66	1.49	1.44
1	2A	1942	5MC	C6-N1	-2.65	1.33	1.38
1	1A	1911	PSU	C4-N3	-2.65	1.33	1.38
54	2x	32	5MC	C6-C5	2.65	1.38	1.34
1	1A	1917	PSU	C4-N3	-2.64	1.33	1.38
32	2a	1518	MA6	C5-C4	2.64	1.47	1.40
1	2A	1939	5MU	C6-N1	-2.64	1.33	1.38
32	1a	1404	5MC	C6-C5	2.62	1.38	1.34
32	2a	1407	5MC	C6-C5	2.58	1.38	1.34
54	2x	54	5MU	C2-N1	2.57	1.42	1.38
54	2x	55	PSU	C4-N3	-2.55	1.34	1.38
32	1a	1518	MA6	C5-C4	2.55	1.47	1.40
32	2a	966	M2G	C6-N1	-2.54	1.34	1.37
54	2x	54	5MU	C4-N3	-2.53	1.34	1.38
32	1a	1519	MA6	C5-C4	2.53	1.47	1.40
1	1A	1939	5MU	C2-N3	-2.53	1.33	1.38
1	1A	1915	5MU	C4-N3	-2.53	1.34	1.38
32	1a	516	PSU	C4-N3	-2.53	1.34	1.38
1	1A	1962	5MC	C6-C5	2.52	1.38	1.34
32	2a	1519	MA6	C5-C4	2.52	1.47	1.40
54	1x	55	PSU	C4-N3	-2.52	1.34	1.38
1	2A	1917	PSU	C4-N3	-2.50	1.34	1.38
54	2x	8	4SU	O2-C2	2.49	1.27	1.23
1	2A	1915	5MU	C4-N3	-2.48	1.34	1.38
32	2a	516	PSU	C4-N3	-2.46	1.34	1.38
1	2A	1911	PSU	C4-N3	-2.44	1.34	1.38
1	2A	1915	5MU	C2-N1	2.38	1.42	1.38
54	1x	32	5MC	C6-N1	-2.37	1.34	1.38
1	2A	1942	5MC	C6-C5	2.36	1.38	1.34
1	1A	1939	5MU	C6-N1	-2.36	1.34	1.38
32	2a	527	7MG	C8-N9	2.35	1.47	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	2251	OMG	C6-N1	-2.34	1.34	1.37
32	2a	1407	5MC	C6-N1	-2.33	1.34	1.38
1	2A	2605	PSU	C2-N3	-2.33	1.33	1.37
54	2x	32	5MC	C6-N1	-2.32	1.34	1.38
54	2x	54	5MU	C4-C5	2.32	1.48	1.44
54	2x	8	4SU	C2-N1	2.32	1.42	1.38
1	1A	2605	PSU	C2-N3	-2.30	1.33	1.37
1	2A	1939	5MU	C2-N3	-2.28	1.33	1.38
32	1a	1498	UR3	C2-N1	2.26	1.41	1.38
1	1A	1962	5MC	C6-N1	-2.26	1.34	1.38
1	2A	2552	2MU	C5-C4	2.26	1.48	1.43
1	2A	1962	5MC	C6-N1	-2.25	1.34	1.38
32	2a	527	7MG	C6-N1	-2.25	1.34	1.38
1	1A	1939	5MU	C4-C5	2.23	1.48	1.44
54	2x	8	4SU	C2-N3	-2.23	1.34	1.38
32	1a	527	7MG	C6-N1	-2.23	1.34	1.38
32	1a	966	M2G	C2-N2	2.23	1.39	1.35
1	2A	2503	2MA	C6-N1	-2.20	1.33	1.38
32	1a	967	5MC	C6-N1	-2.20	1.34	1.38
32	2a	1400	5MC	C6-N1	-2.19	1.34	1.38
1	2A	2552	2MU	C2-N3	-2.18	1.34	1.38
32	1a	527	7MG	C8-N9	2.16	1.47	1.46
1	1A	1942	5MC	C6-N1	-2.15	1.34	1.38
1	2A	1911	PSU	C2-N1	-2.12	1.33	1.36
1	1A	2552	2MU	C2-N3	-2.12	1.34	1.38
54	1x	54	5MU	C2-N3	-2.12	1.34	1.38
32	1a	1404	5MC	C6-N1	-2.09	1.34	1.38
54	1x	54	5MU	C2-N1	2.08	1.41	1.38
32	1a	1400	5MC	C6-N1	-2.07	1.34	1.38
1	2A	1915	5MU	C6-N1	-2.05	1.34	1.38
54	1x	54	5MU	C6-N1	-2.04	1.34	1.38
32	2a	1404	5MC	C6-N1	-2.04	1.34	1.38
1	2A	1915	5MU	C2-N3	-2.02	1.34	1.38
1	1A	1911	PSU	C2-N3	-2.01	1.34	1.37

All (194) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	2l	92	0TD	CSB-SB-CB	-22.92	60.97	102.44
32	1a	527	7MG	N9-C4-N3	8.63	138.37	125.47
32	2a	527	7MG	N9-C4-N3	8.30	137.89	125.47
43	1l	92	0TD	CSB-SB-CB	7.34	115.72	102.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	1498	UR3	C4-N3-C2	-6.48	118.47	124.56
1	2A	1917	PSU	N1-C2-N3	6.19	122.14	115.13
32	1a	1498	UR3	C4-N3-C2	-6.13	118.80	124.56
1	2A	1939	5MU	C4-N3-C2	-5.91	119.70	127.35
1	1A	1911	PSU	N1-C2-N3	5.83	121.74	115.13
54	1x	55	PSU	N1-C2-N3	5.81	121.72	115.13
32	2a	516	PSU	N1-C2-N3	5.74	121.64	115.13
32	1a	516	PSU	N1-C2-N3	5.74	121.64	115.13
1	1A	1917	PSU	N1-C2-N3	5.66	121.55	115.13
1	2A	2605	PSU	N1-C2-N3	5.64	121.52	115.13
54	2x	55	PSU	N1-C2-N3	5.61	121.49	115.13
1	2A	1911	PSU	N1-C2-N3	5.60	121.47	115.13
1	2A	1939	5MU	N3-C2-N1	5.45	122.12	114.89
32	1a	527	7MG	C5-C4-N3	-5.35	117.94	128.13
1	1A	2552	2MU	N3-C2-N1	5.26	121.87	114.89
32	2a	527	7MG	N9-C8-N7	-5.23	95.90	103.38
1	2A	2552	2MU	N3-C2-N1	5.23	121.83	114.89
1	2A	1915	5MU	C4-N3-C2	-5.18	120.64	127.35
1	1A	2605	PSU	N1-C2-N3	5.18	121.00	115.13
32	2a	527	7MG	C5-C4-N3	-5.12	118.38	128.13
1	1A	1915	5MU	C4-N3-C2	-5.04	120.82	127.35
1	2A	1915	5MU	N3-C2-N1	4.98	121.50	114.89
1	1A	1915	5MU	N3-C2-N1	4.98	121.50	114.89
1	1A	1939	5MU	C4-N3-C2	-4.96	120.92	127.35
1	2A	1939	5MU	C5-C6-N1	-4.95	118.25	123.34
1	1A	1939	5MU	N3-C2-N1	4.88	121.37	114.89
32	1a	527	7MG	N9-C8-N7	-4.84	96.45	103.38
54	2x	54	5MU	C4-N3-C2	-4.81	121.12	127.35
54	2x	54	5MU	N3-C2-N1	4.81	121.27	114.89
54	1x	8	4SU	C5-C4-N3	4.79	119.13	114.69
54	1x	54	5MU	N3-C2-N1	4.79	121.25	114.89
1	2A	1915	5MU	C5-C4-N3	4.76	119.37	115.31
1	2A	1939	5MU	C5-C4-N3	4.70	119.32	115.31
1	2A	2552	2MU	C4-N3-C2	-4.64	120.45	126.58
54	2x	8	4SU	C1'-N1-C2	4.60	125.90	117.57
1	1A	1915	5MU	C5-C4-N3	4.58	119.22	115.31
1	1A	2552	2MU	C4-N3-C2	-4.44	120.72	126.58
54	2x	54	5MU	C5-C4-N3	4.43	119.09	115.31
54	1x	54	5MU	C4-N3-C2	-4.41	121.64	127.35
54	2x	54	5MU	O4-C4-C5	-4.29	119.93	124.90
1	1A	1939	5MU	C5-C6-N1	-4.27	118.94	123.34
1	1A	1939	5MU	C5-C4-N3	4.26	118.94	115.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	527	7MG	C2-N3-C4	4.16	119.71	112.30
54	1x	32	5MC	C5-C6-N1	-4.16	119.06	123.34
32	1a	527	7MG	C2-N3-C4	4.06	119.53	112.30
54	1x	55	PSU	C4-N3-C2	-4.04	120.52	126.34
1	2A	1917	PSU	C4-N3-C2	-4.03	120.54	126.34
1	2A	2605	PSU	C4-N3-C2	-3.91	120.70	126.34
1	1A	1911	PSU	C4-N3-C2	-3.86	120.77	126.34
1	2A	1911	PSU	O2-C2-N1	-3.85	118.56	122.79
54	1x	54	5MU	C5-C4-N3	3.76	118.52	115.31
32	2a	516	PSU	C4-N3-C2	-3.74	120.94	126.34
54	2x	55	PSU	C4-N3-C2	-3.74	120.95	126.34
1	1A	1917	PSU	C4-N3-C2	-3.74	120.95	126.34
1	1A	1915	5MU	O4-C4-C5	-3.73	120.57	124.90
32	2a	1518	MA6	C9-N6-C6	-3.71	108.27	119.51
1	2A	1915	5MU	O4-C4-C5	-3.68	120.63	124.90
54	1x	54	5MU	O4-C4-C5	-3.64	120.68	124.90
32	1a	516	PSU	C4-N3-C2	-3.55	121.23	126.34
32	1a	1519	MA6	N1-C6-N6	3.50	120.74	117.06
1	2A	1911	PSU	C4-N3-C2	-3.50	121.30	126.34
54	2x	8	4SU	C6-C5-C4	-3.47	116.94	119.95
1	1A	1939	5MU	O4-C4-C5	-3.46	120.89	124.90
32	1a	1404	5MC	C5-C6-N1	-3.45	119.79	123.34
1	1A	2605	PSU	C4-N3-C2	-3.45	121.37	126.34
32	2a	1519	MA6	C9-N6-C6	-3.43	109.14	119.51
1	1A	2552	2MU	O2-C2-N1	-3.42	118.25	122.79
32	2a	967	5MC	C5-C6-N1	-3.42	119.82	123.34
32	1a	967	5MC	C5-C6-N1	-3.39	119.85	123.34
32	2a	1400	5MC	C5-C6-N1	-3.38	119.86	123.34
32	2a	1518	MA6	C4-C5-N7	-3.35	105.90	109.40
32	2a	1518	MA6	N3-C2-N1	-3.35	123.44	128.68
54	1x	8	4SU	C6-C5-C4	-3.35	117.05	119.95
1	2A	1962	5MC	C5-C6-N1	-3.30	119.94	123.34
1	1A	1942	5MC	C5-C6-N1	-3.30	119.94	123.34
1	2A	1939	5MU	O2-C2-N1	-3.30	118.40	122.79
32	1a	1518	MA6	C9-N6-C6	-3.30	109.53	119.51
32	2a	1404	5MC	C5-C6-N1	-3.28	119.97	123.34
32	2a	1519	MA6	C4-C5-N7	-3.25	106.02	109.40
1	2A	1942	5MC	C5-C6-N1	-3.23	120.01	123.34
32	2a	516	PSU	O2-C2-N1	-3.22	119.24	122.79
1	2A	1915	5MU	C5-C6-N1	-3.22	120.03	123.34
1	2A	1939	5MU	O4-C4-C5	-3.22	121.17	124.90
54	1x	54	5MU	C5-C6-N1	-3.21	120.03	123.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	2x	8	4SU	C5-C4-N3	3.21	117.67	114.69
32	1a	1518	MA6	N3-C2-N1	-3.18	123.70	128.68
32	1a	1518	MA6	C4-C5-N7	-3.17	106.10	109.40
1	2A	1917	PSU	O2-C2-N1	-3.15	119.32	122.79
32	1a	1519	MA6	C9-N6-C6	-3.14	110.00	119.51
32	1a	1519	MA6	N3-C2-N1	-3.13	123.78	128.68
1	1A	1962	5MC	C5-C6-N1	-3.11	120.14	123.34
1	1A	1911	PSU	O2-C2-N1	-3.10	119.38	122.79
54	1x	32	5MC	C5-C4-N3	-3.09	118.34	121.67
32	1a	1400	5MC	C5-C6-N1	-3.07	120.18	123.34
43	1l	92	0TD	OD2-CG-CB	3.06	119.77	113.15
32	2a	1407	5MC	C5-C4-N3	-3.06	118.38	121.67
54	2x	54	5MU	C5-C6-N1	-3.05	120.20	123.34
32	1a	1407	5MC	C5-C4-N3	-3.01	118.43	121.67
32	1a	516	PSU	O2-C2-N1	-3.01	119.48	122.79
32	2a	1519	MA6	N3-C2-N1	-3.01	123.97	128.68
32	1a	1407	5MC	C5-C6-N1	-3.00	120.26	123.34
54	2x	55	PSU	O2-C2-N1	-2.98	119.51	122.79
1	1A	1915	5MU	C5-C6-N1	-2.98	120.28	123.34
54	1x	55	PSU	O2-C2-N1	-2.98	119.52	122.79
1	1A	2552	2MU	O4-C4-C5	-2.94	119.99	125.16
1	1A	2552	2MU	C5-C4-N3	2.93	119.22	114.84
1	2A	1962	5MC	C5-C4-N3	-2.92	118.53	121.67
32	2a	1400	5MC	C5-C4-N3	-2.88	118.56	121.67
1	2A	2552	2MU	O2-C2-N1	-2.87	118.97	122.79
32	1a	1207	2MG	CM2-N2-C2	-2.81	117.66	123.86
1	2A	2552	2MU	C5-C4-N3	2.80	119.03	114.84
1	1A	2552	2MU	C2'-C1'-N1	-2.77	108.85	114.22
32	1a	1400	5MC	C5-C4-N3	-2.71	118.75	121.67
54	2x	32	5MC	C5-C6-N1	-2.70	120.56	123.34
32	2a	1407	5MC	C5-C6-N1	-2.66	120.60	123.34
32	1a	1518	MA6	C10-N6-C9	-2.63	107.65	116.12
1	1A	1917	PSU	O2-C2-N1	-2.63	119.90	122.79
1	2A	2605	PSU	O2-C2-N1	-2.63	119.90	122.79
54	2x	32	5MC	C5-C4-N3	-2.61	118.85	121.67
32	1a	1519	MA6	C4-C5-N7	-2.60	106.69	109.40
1	1A	1915	5MU	C5M-C5-C4	2.57	121.60	118.77
1	2A	2251	OMG	O6-C6-C5	-2.55	119.38	124.37
1	2A	1920	4OC	O2-C2-N3	-2.55	118.19	122.33
32	2a	527	7MG	C5-C6-N1	2.55	115.48	110.99
32	1a	1518	MA6	N1-C6-N6	2.54	119.73	117.06
1	1A	1942	5MC	C5-C4-N3	-2.50	118.97	121.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	1962	5MC	C5-C4-N3	-2.50	118.97	121.67
1	1A	2251	OMG	C5-C6-N1	2.48	118.33	113.95
32	1a	1400	5MC	O2-C2-N3	-2.47	118.31	122.33
32	1a	527	7MG	C5-C6-N1	2.46	115.32	110.99
1	1A	2605	PSU	O2-C2-N1	-2.46	120.09	122.79
54	1x	55	PSU	C5-C6-N1	-2.44	118.45	122.11
1	2A	1942	5MC	C5-C4-N3	-2.43	119.05	121.67
1	2A	2503	2MA	C5-C6-N1	2.42	118.20	114.02
54	2x	54	5MU	O2-C2-N1	-2.41	119.58	122.79
32	1a	1207	2MG	C5-C6-N1	2.41	118.20	113.95
32	2a	1404	5MC	C5-C4-N3	-2.41	119.08	121.67
1	1A	2605	PSU	C6-C5-C4	-2.38	116.53	118.20
1	1A	2503	2MA	C8-N7-C5	2.38	107.52	102.99
32	2a	967	5MC	C5-C4-N3	-2.37	119.11	121.67
1	2A	2552	2MU	O4-C4-C5	-2.37	121.00	125.16
1	2A	1915	5MU	C5M-C5-C4	2.36	121.37	118.77
32	1a	1207	2MG	C8-N7-C5	2.35	107.47	102.99
1	2A	1939	5MU	C5M-C5-C6	-2.33	119.73	122.85
1	2A	1962	5MC	O2-C2-N3	-2.33	118.54	122.33
32	2a	967	5MC	O2-C2-N3	-2.32	118.56	122.33
1	2A	2503	2MA	C8-N7-C5	2.32	107.40	102.99
32	2a	1207	2MG	C8-N7-C5	2.30	107.38	102.99
1	2A	1939	5MU	C5M-C5-C4	2.30	121.30	118.77
54	2x	8	4SU	C6-N1-C2	-2.28	118.07	120.99
1	2A	2251	OMG	C5-C6-N1	2.27	117.96	113.95
1	2A	1920	4OC	C1'-N1-C2	2.27	123.48	118.42
32	1a	966	M2G	C5-C6-N1	2.26	117.94	113.95
32	2a	1518	MA6	C10-N6-C6	-2.23	112.75	119.51
1	2A	2552	2MU	C2'-C1'-N1	-2.23	109.89	114.22
54	2x	8	4SU	C1'-N1-C6	-2.22	115.99	120.84
32	1a	1404	5MC	O2-C2-N3	-2.22	118.72	122.33
1	1A	2503	2MA	C5-C6-N1	2.22	117.84	114.02
32	2a	1518	MA6	C10-N6-C9	-2.21	109.00	116.12
32	1a	1404	5MC	C5-C4-N3	-2.21	119.29	121.67
32	1a	967	5MC	C5-C4-N3	-2.20	119.30	121.67
54	1x	54	5MU	O2-C2-N1	-2.20	119.86	122.79
1	1A	1915	5MU	C1'-N1-C2	2.20	121.55	117.57
32	2a	516	PSU	O4'-C1'-C2'	2.19	108.24	105.14
32	1a	1404	5MC	C1'-N1-C6	-2.17	117.51	121.12
32	2a	966	M2G	C8-N7-C5	2.17	107.13	102.99
54	1x	32	5MC	N1-C2-N3	2.17	122.76	118.81
32	1a	1400	5MC	CM5-C5-C6	-2.17	119.95	122.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	1a	1402	4OC	CM4-N4-C4	-2.17	118.22	122.45
32	1a	1404	5MC	CM5-C5-C6	-2.16	119.97	122.85
32	1a	967	5MC	O2-C2-N3	-2.16	118.82	122.33
32	1a	1519	MA6	C10-N6-C6	-2.14	113.04	119.51
32	2a	527	7MG	CM7-N7-C5	2.13	131.89	126.40
32	2a	1519	MA6	C10-N6-C6	-2.11	113.12	119.51
32	2a	1207	2MG	CM2-N2-C2	-2.10	119.22	123.86
1	1A	1920	4OC	O2-C2-N3	-2.09	118.93	122.33
32	1a	966	M2G	C8-N7-C5	2.09	106.97	102.99
54	2x	8	4SU	O2-C2-N1	2.09	125.56	122.79
32	2a	1400	5MC	O2-C2-N3	-2.06	118.98	122.33
1	2A	1915	5MU	O2-C2-N1	-2.06	120.05	122.79
32	1a	527	7MG	CM7-N7-C5	2.05	131.70	126.40
32	1a	527	7MG	C5-C4-N9	-2.05	103.69	106.35
54	1x	32	5MC	O2-C2-N3	-2.04	119.01	122.33
32	2a	1407	5MC	O2-C2-N3	-2.04	119.02	122.33
32	2a	1498	UR3	C3U-N3-C4	2.03	120.80	117.89
32	2a	527	7MG	C5-C4-N9	-2.03	103.71	106.35
32	1a	1498	UR3	C1'-N1-C2	2.02	120.41	116.99
32	2a	1402	4OC	C6-C5-C4	2.01	119.42	116.96
54	2x	55	PSU	C5-C6-N1	-2.00	119.10	122.11
1	1A	2251	OMG	C8-N7-C5	2.00	106.81	102.99

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1A	1915	5MU	C3'-C4'-C5'-O5'
32	1a	1518	MA6	C5-C6-N6-C9
32	1a	1518	MA6	C5-C6-N6-C10
32	1a	1519	MA6	O4'-C4'-C5'-O5'
1	2A	2251	OMG	C1'-C2'-O2'-CM2
32	2a	966	M2G	N1-C2-N2-CM2
32	2a	966	M2G	N3-C2-N2-CM1
32	2a	966	M2G	N3-C2-N2-CM2
32	2a	1400	5MC	O4'-C4'-C5'-O5'
32	2a	1402	4OC	O4'-C4'-C5'-O5'
32	2a	1402	4OC	C3'-C4'-C5'-O5'
32	2a	1518	MA6	C5-C6-N6-C10
32	2a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
32	2a	1519	MA6	C5-C6-N6-C10

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Mol	Chain	Res	Type	Atoms
43	2l	92	0TD	CA-CB-SB-CSB
43	2l	92	0TD	CG-CB-SB-CSB
1	1A	1915	5MU	O4'-C4'-C5'-O5'
32	1a	527	7MG	C3'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
32	2a	1400	5MC	C3'-C4'-C5'-O5'
32	1a	527	7MG	O4'-C4'-C5'-O5'
32	1a	1519	MA6	C5-C6-N6-C10
32	2a	1518	MA6	C5-C6-N6-C9
32	2a	1519	MA6	C5-C6-N6-C9
32	1a	1518	MA6	N1-C6-N6-C9
32	2a	527	7MG	C3'-C4'-C5'-O5'
32	2a	966	M2G	N1-C2-N2-CM1
32	1a	1402	4OC	C1'-C2'-O2'-CM2
32	1a	1402	4OC	O4'-C4'-C5'-O5'
43	2l	92	0TD	SB-CB-CG-OD1
32	1a	967	5MC	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C4'-C5'-O5'-P
32	2a	527	7MG	O4'-C4'-C5'-O5'
32	1a	1519	MA6	C4'-C5'-O5'-P
32	1a	1402	4OC	C3'-C2'-O2'-CM2
1	1A	2503	2MA	O4'-C4'-C5'-O5'
1	2A	1920	4OC	C2'-C1'-N1-C6
32	2a	1518	MA6	N1-C6-N6-C9
1	2A	1962	5MC	C2'-C1'-N1-C6
43	1l	92	0TD	CA-CB-SB-CSB
1	2A	1920	4OC	C2'-C1'-N1-C2
1	2A	2552	2MU	O4'-C4'-C5'-O5'
1	2A	1962	5MC	O4'-C1'-N1-C6
32	2a	1402	4OC	C2'-C1'-N1-C6
1	2A	1911	PSU	O4'-C4'-C5'-O5'
43	1l	92	0TD	CG-CB-SB-CSB
32	1a	1402	4OC	C3'-C4'-C5'-O5'
1	2A	2503	2MA	O4'-C4'-C5'-O5'
43	1l	92	0TD	SB-CB-CG-OD1
32	2a	1402	4OC	C2'-C1'-N1-C2
1	1A	2503	2MA	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 2563 ligands modelled in this entry, 2561 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
58	SF4	1d	501	35	0,12,12	-	-	-		
58	SF4	2d	302	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
58	SF4	1d	501	35	-	-	0/6/5/5
58	SF4	2d	302	35	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.25	16 (0%) 89 72	28, 46, 94, 110	0
1	2A	2789/2915 (95%)	0.18	27 (0%) 82 59	39, 62, 93, 108	0
2	1B	120/121 (99%)	-0.05	0 100 100	37, 56, 68, 89	0
2	2B	120/121 (99%)	0.06	3 (2%) 57 29	62, 80, 90, 95	0
3	1D	275/276 (99%)	0.54	7 (2%) 57 29	30, 47, 59, 71	0
3	2D	275/276 (99%)	0.65	30 (10%) 5 2	40, 56, 69, 75	0
4	1E	204/206 (99%)	0.23	7 (3%) 45 19	33, 47, 62, 76	0
4	2E	204/206 (99%)	0.53	19 (9%) 8 3	41, 62, 71, 78	0
5	1F	203/210 (96%)	-0.01	0 100 100	31, 49, 67, 83	0
5	2F	203/210 (96%)	0.03	7 (3%) 45 19	46, 66, 79, 85	0
6	1G	181/182 (99%)	-0.08	0 100 100	44, 60, 71, 85	0
6	2G	181/182 (99%)	0.49	17 (9%) 8 3	69, 80, 87, 93	0
7	1H	174/180 (96%)	-0.12	0 100 100	43, 58, 69, 75	0
7	2H	174/180 (96%)	-0.01	4 (2%) 60 31	66, 79, 88, 95	0
8	1I	146/148 (98%)	-0.20	0 100 100	48, 70, 78, 85	0
8	2I	146/148 (98%)	-0.14	4 (2%) 54 26	59, 75, 84, 89	0
9	1N	140/140 (100%)	0.01	0 100 100	35, 48, 62, 70	0
9	2N	140/140 (100%)	0.74	18 (12%) 3 1	51, 66, 80, 87	0
10	1O	122/122 (100%)	0.19	0 100 100	36, 50, 62, 68	0
10	2O	122/122 (100%)	0.13	1 (0%) 86 65	48, 58, 68, 73	0
11	1P	149/150 (99%)	0.22	3 (2%) 65 36	33, 52, 68, 74	0
11	2P	149/150 (99%)	0.47	17 (11%) 5 1	42, 66, 79, 84	0
12	1Q	141/141 (100%)	0.44	1 (0%) 87 69	38, 50, 60, 66	0
12	2Q	141/141 (100%)	0.46	6 (4%) 35 13	51, 65, 75, 83	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	1R	118/118 (100%)	0.24	1 (0%) 86 65	35, 44, 56, 67	0
13	2R	118/118 (100%)	1.18	32 (27%) 0 0	48, 58, 67, 77	0
14	1S	110/112 (98%)	0.01	0 100 100	44, 53, 62, 66	0
14	2S	110/112 (98%)	0.42	13 (11%) 4 1	62, 74, 82, 87	0
15	1T	131/146 (89%)	0.01	0 100 100	41, 53, 69, 82	0
15	2T	131/146 (89%)	0.21	6 (4%) 32 12	52, 62, 75, 83	0
16	1U	116/118 (98%)	0.41	4 (3%) 45 19	33, 42, 54, 69	0
16	2U	116/118 (98%)	0.44	3 (2%) 56 27	48, 64, 74, 82	0
17	1V	101/101 (100%)	0.01	0 100 100	33, 47, 63, 74	0
17	2V	101/101 (100%)	-0.07	3 (2%) 50 22	54, 68, 78, 86	0
18	1W	112/113 (99%)	0.08	0 100 100	34, 42, 56, 77	0
18	2W	112/113 (99%)	0.44	3 (2%) 54 26	43, 55, 68, 76	0
19	1X	95/96 (98%)	0.26	1 (1%) 80 56	34, 46, 61, 78	0
19	2X	95/96 (98%)	0.75	5 (5%) 26 10	48, 66, 77, 80	0
20	1Y	107/110 (97%)	-0.09	1 (0%) 84 63	41, 54, 70, 77	0
20	2Y	107/110 (97%)	0.69	15 (14%) 2 1	61, 72, 79, 87	0
21	1Z	154/206 (74%)	-0.23	0 100 100	45, 62, 74, 83	0
21	2Z	160/206 (77%)	-0.28	0 100 100	64, 75, 83, 87	0
22	10	76/85 (89%)	0.37	0 100 100	37, 47, 56, 61	0
22	20	76/85 (89%)	1.62	31 (40%) 0 0	55, 64, 71, 79	0
23	11	97/98 (98%)	0.43	3 (3%) 49 21	36, 51, 70, 80	0
23	21	97/98 (98%)	0.93	17 (17%) 1 0	48, 62, 75, 77	0
24	12	70/72 (97%)	-0.12	0 100 100	40, 54, 63, 72	0
24	22	70/72 (97%)	0.27	3 (4%) 35 13	60, 71, 77, 79	0
25	13	59/60 (98%)	0.10	0 100 100	37, 45, 62, 71	0
25	23	59/60 (98%)	0.86	6 (10%) 6 2	53, 66, 79, 88	0
26	14	69/71 (97%)	-0.42	0 100 100	57, 73, 84, 94	0
26	24	69/71 (97%)	-0.33	4 (5%) 23 7	70, 83, 91, 95	0
27	15	59/60 (98%)	0.30	0 100 100	33, 42, 57, 71	0
27	25	59/60 (98%)	0.32	1 (1%) 70 41	48, 56, 67, 71	0
28	16	53/54 (98%)	0.02	1 (1%) 66 37	40, 47, 57, 63	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	26	53/54 (98%)	0.13	0 100 100	55, 62, 72, 79	0
29	17	48/49 (97%)	0.88	5 (10%) 6 2	32, 41, 60, 69	0
29	27	48/49 (97%)	1.15	8 (16%) 1 0	45, 51, 73, 80	0
30	18	64/65 (98%)	0.83	8 (12%) 3 1	34, 43, 52, 64	0
30	28	64/65 (98%)	1.40	16 (25%) 0 0	49, 59, 67, 73	0
31	19	37/37 (100%)	1.05	6 (16%) 1 0	39, 50, 66, 73	0
31	29	37/37 (100%)	1.66	14 (37%) 0 0	61, 68, 78, 80	0
32	1a	1488/1521 (97%)	0.23	62 (4%) 36 14	44, 72, 92, 106	0
32	2a	1491/1521 (98%)	0.30	86 (5%) 23 7	56, 77, 95, 106	0
33	1b	231/256 (90%)	-0.42	0 100 100	65, 77, 87, 92	0
33	2b	231/256 (90%)	-0.09	8 (3%) 44 18	67, 83, 89, 95	0
34	1c	206/239 (86%)	0.11	15 (7%) 15 4	63, 74, 82, 90	0
34	2c	206/239 (86%)	0.04	13 (6%) 20 6	66, 81, 89, 92	0
35	1d	208/209 (99%)	0.69	25 (12%) 4 1	62, 73, 81, 91	0
35	2d	208/209 (99%)	0.21	4 (1%) 66 37	62, 74, 80, 86	0
36	1e	148/162 (91%)	0.34	10 (6%) 17 5	56, 68, 77, 80	0
36	2e	148/162 (91%)	0.44	12 (8%) 12 3	63, 74, 81, 88	0
37	1f	100/101 (99%)	-0.30	0 100 100	58, 70, 78, 79	0
37	2f	100/101 (99%)	-0.41	0 100 100	56, 70, 80, 82	0
38	1g	155/156 (99%)	-0.06	6 (3%) 39 15	64, 72, 83, 88	0
38	2g	155/156 (99%)	0.22	15 (9%) 7 2	70, 79, 90, 104	0
39	1h	137/138 (99%)	0.44	12 (8%) 10 3	61, 69, 76, 81	0
39	2h	137/138 (99%)	0.69	23 (16%) 1 0	65, 75, 82, 86	0
40	1i	127/128 (99%)	1.02	28 (22%) 0 0	60, 76, 82, 86	0
40	2i	127/128 (99%)	1.84	47 (37%) 0 0	69, 83, 90, 92	0
41	1j	97/105 (92%)	0.94	25 (25%) 0 0	64, 78, 86, 93	0
41	2j	96/105 (91%)	1.11	26 (27%) 0 0	71, 84, 90, 92	0
42	1k	114/129 (88%)	-0.17	0 100 100	53, 69, 80, 82	0
42	2k	114/129 (88%)	-0.09	2 (1%) 68 40	64, 73, 79, 84	0
43	1l	121/132 (91%)	0.27	11 (9%) 9 3	53, 64, 73, 77	0
43	2l	121/132 (91%)	0.57	17 (14%) 2 1	58, 67, 76, 84	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	1m	123/126 (97%)	0.26	15 (12%) 4 1	62, 72, 80, 94	0
44	2m	122/126 (96%)	1.07	27 (22%) 0 0	71, 80, 86, 102	0
45	1n	60/61 (98%)	2.67	38 (63%) 0 0	65, 72, 78, 81	0
45	2n	60/61 (98%)	2.93	39 (65%) 0 0	72, 82, 88, 91	0
46	1o	88/89 (98%)	0.00	0 100 100	55, 66, 79, 84	0
46	2o	88/89 (98%)	0.33	3 (3%) 45 19	62, 71, 79, 84	0
47	1p	82/88 (93%)	1.90	34 (41%) 0 0	59, 75, 83, 87	0
47	2p	82/88 (93%)	0.72	12 (14%) 2 1	60, 70, 79, 83	0
48	1q	99/105 (94%)	0.60	11 (11%) 5 1	58, 68, 78, 82	0
48	2q	99/105 (94%)	1.28	25 (25%) 0 0	57, 71, 77, 80	0
49	1r	68/88 (77%)	-0.18	1 (1%) 73 46	62, 71, 78, 83	0
49	2r	68/88 (77%)	-0.37	0 100 100	64, 71, 76, 82	0
50	1s	83/93 (89%)	-0.25	1 (1%) 79 54	64, 75, 82, 84	0
50	2s	83/93 (89%)	0.67	12 (14%) 2 1	75, 84, 90, 95	0
51	1t	96/106 (90%)	0.73	19 (19%) 1 0	61, 70, 78, 82	0
51	2t	96/106 (90%)	1.01	23 (23%) 0 0	56, 71, 79, 81	0
52	1u	23/27 (85%)	2.30	13 (56%) 0 0	64, 70, 73, 76	0
52	2u	23/27 (85%)	3.07	17 (73%) 0 0	73, 79, 84, 86	0
53	1v	13/24 (54%)	3.29	5 (38%) 0 0	53, 92, 100, 103	0
53	2v	13/24 (54%)	4.05	7 (53%) 0 0	72, 97, 102, 103	0
54	1x	72/77 (93%)	-0.18	0 100 100	46, 66, 82, 88	0
54	2x	72/77 (93%)	-0.37	0 100 100	56, 77, 89, 94	0
55	1z	16/16 (100%)	0.47	1 (6%) 20 6	38, 47, 62, 71	0
55	2z	16/16 (100%)	1.81	4 (25%) 0 0	52, 58, 66, 72	0
All	All	20628/21476 (96%)	0.30	1151 (5%) 24 8	28, 66, 87, 110	0

All (1151) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
44	2m	124	PRO	17.8
53	1v	24	A	14.0
53	2v	24	A	11.9
52	2u	14	TRP	9.8
44	2m	102	ARG	9.2

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Mol	Chain	Res	Type	RSRZ
38	2g	82	GLY	9.1
40	2i	124	GLN	8.3
53	2v	23	A	8.3
23	21	2	SER	8.1
40	2i	123	PRO	7.9
44	2m	123	ALA	7.9
40	2i	125	TYR	7.8
39	2h	2	LEU	7.7
45	2n	2	ALA	7.7
44	1m	124	PRO	7.5
41	2j	55	LYS	7.4
53	1v	23	A	7.4
40	1i	117	HIS	7.3
40	2i	119	ALA	7.3
29	27	48	LYS	7.2
40	1i	114	TYR	7.2
32	1a	1257	U	7.0
41	1j	62	HIS	6.9
41	1j	60	ARG	6.9
32	2a	1532	U	6.9
44	2m	120	LYS	6.9
55	2z	13	PRO	6.8
45	1n	32	SER	6.8
41	1j	63	PHE	6.7
31	29	37	GLY	6.6
40	2i	115	GLY	6.5
45	1n	21	TYR	6.5
41	1j	47	PHE	6.5
40	2i	127	LYS	6.4
47	1p	7	ALA	6.3
53	2v	21	C	6.3
52	1u	14	TRP	6.3
40	2i	110	GLU	6.3
45	2n	25	VAL	6.3
22	20	76	GLY	6.2
41	2j	46	ARG	6.2
53	2v	22	U	6.2
41	1j	59	SER	6.1
29	17	46	VAL	6.1
32	1a	1367	C	6.1
44	2m	106	ASN	6.1
40	2i	116	LYS	6.0

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Mol	Chain	Res	Type	RSRZ
41	2j	49	VAL	6.0
41	2j	58	ASP	6.0
13	2R	69	ASP	5.9
45	2n	34	TYR	5.9
53	1v	22	U	5.9
45	1n	22	THR	5.8
45	2n	39	LEU	5.8
44	1m	106	ASN	5.8
47	1p	6	LEU	5.7
40	2i	106	ALA	5.6
39	2h	93	VAL	5.6
45	1n	58	LYS	5.6
41	1j	58	ASP	5.6
44	2m	90	LEU	5.6
34	2c	4	LYS	5.5
40	2i	14	VAL	5.5
45	2n	33	VAL	5.5
40	1i	115	GLY	5.4
44	2m	100	GLY	5.4
45	1n	61	TRP	5.4
45	2n	11	LYS	5.4
40	2i	113	LYS	5.4
41	2j	47	PHE	5.4
41	2j	67	THR	5.4
48	2q	32	TYR	5.3
20	2Y	1	MET	5.3
29	17	45	ALA	5.3
40	1i	113	LYS	5.2
36	2e	88	LYS	5.2
40	2i	117	HIS	5.2
40	2i	126	SER	5.2
40	1i	109	VAL	5.2
43	2l	18	VAL	5.2
45	2n	61	TRP	5.1
47	1p	19	ILE	5.1
40	1i	110	GLU	5.1
53	2v	12	A	5.1
41	1j	64	GLU	5.1
42	2k	126	ARG	5.1
52	2u	6	ARG	5.1
41	1j	46	ARG	5.0
41	2j	50	ILE	5.0

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Mol	Chain	Res	Type	RSRZ
52	2u	17	THR	5.0
32	1a	1357	A	5.0
52	2u	16	GLY	5.0
51	2t	25	ARG	4.9
44	2m	6	GLY	4.9
29	17	48	LYS	4.9
32	1a	975	A	4.9
44	2m	105	THR	4.9
38	2g	33	ASP	4.9
45	2n	18	VAL	4.8
41	2j	60	ARG	4.8
48	2q	35	VAL	4.8
32	1a	1366	C	4.8
41	1j	57	LYS	4.8
32	1a	1356	G	4.8
45	2n	22	THR	4.8
40	2i	9	ARG	4.7
41	2j	48	THR	4.7
48	2q	8	GLY	4.7
45	1n	2	ALA	4.7
38	2g	80	VAL	4.7
51	2t	80	ARG	4.7
45	1n	59	ALA	4.7
45	1n	35	ARG	4.7
45	2n	7	ILE	4.7
51	2t	9	ASN	4.6
45	2n	41	ARG	4.6
32	2a	973	G	4.6
41	1j	49	VAL	4.6
6	2G	28	VAL	4.6
52	1u	18	TYR	4.6
32	1a	1368	G	4.6
45	2n	35	ARG	4.6
19	2X	92	LEU	4.6
41	1j	48	THR	4.6
40	2i	128	ARG	4.6
40	2i	66	ARG	4.5
40	1i	126	SER	4.5
5	2F	56	GLU	4.5
45	1n	33	VAL	4.5
45	2n	59	ALA	4.5
47	1p	27	LYS	4.5

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Mol	Chain	Res	Type	RSRZ
52	1u	17	THR	4.5
40	1i	118	LYS	4.5
53	2v	13	A	4.5
40	1i	111	ARG	4.5
45	2n	42	ILE	4.5
45	2n	29	ARG	4.5
52	1u	3	LYS	4.4
22	20	55	ARG	4.4
35	2d	68	TYR	4.4
38	2g	79	ARG	4.4
1	2A	1026	U	4.4
48	2q	31	LEU	4.4
40	1i	116	LYS	4.4
53	2v	20	U	4.4
47	1p	4	ILE	4.4
6	2G	94	LEU	4.3
51	1t	21	LYS	4.3
13	2R	5	LYS	4.3
41	2j	59	SER	4.3
39	1h	4	ASP	4.3
41	1j	65	LEU	4.3
41	2j	62	HIS	4.3
40	1i	123	PRO	4.3
40	2i	114	TYR	4.3
45	1n	23	ARG	4.3
40	1i	112	LYS	4.3
41	2j	57	LYS	4.2
51	2t	70	SER	4.2
40	1i	120	ARG	4.2
52	1u	6	ARG	4.2
40	2i	65	VAL	4.2
51	1t	18	GLN	4.2
40	2i	109	VAL	4.2
32	2a	1224	G	4.2
51	1t	70	SER	4.2
44	2m	103	THR	4.2
3	1D	276	LYS	4.1
48	2q	30	PRO	4.1
40	1i	119	ALA	4.1
40	1i	122	ALA	4.1
40	1i	121	ARG	4.1
22	20	43	THR	4.1

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Mol	Chain	Res	Type	RSRZ
53	1v	13	A	4.1
6	2G	34	LEU	4.1
44	1m	111	LYS	4.1
4	2E	151	TYR	4.1
44	2m	122	LYS	4.1
48	2q	38	ARG	4.1
45	2n	30	ALA	4.1
34	2c	2	GLY	4.1
44	2m	104	ARG	4.1
32	1a	1365	G	4.1
12	1Q	33	GLY	4.0
24	22	1	MET	4.0
44	2m	101	GLN	4.0
47	1p	29	ASP	4.0
45	2n	32	SER	4.0
10	2O	1	MET	4.0
22	20	52	GLY	4.0
23	21	15	ALA	4.0
52	2u	13	ILE	4.0
43	2l	5	PRO	4.0
22	20	57	PHE	4.0
48	2q	34	LYS	4.0
31	29	12	ASP	4.0
40	2i	68	GLY	4.0
50	2s	49	ILE	4.0
32	2a	1202	G	3.9
41	1j	50	ILE	3.9
48	2q	36	ILE	3.9
35	1d	70	ILE	3.9
40	1i	125	TYR	3.9
45	1n	17	LYS	3.9
45	1n	11	LYS	3.9
11	2P	45	LEU	3.9
48	2q	37	LYS	3.9
40	2i	69	GLY	3.9
47	1p	18	ARG	3.9
32	1a	976	G	3.9
38	2g	37	ASN	3.9
6	2G	89	GLY	3.8
38	2g	36	LYS	3.8
45	1n	18	VAL	3.8
40	2i	36	TYR	3.8

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Mol	Chain	Res	Type	RSRZ
13	2R	68	ARG	3.8
40	2i	107	ARG	3.8
40	2i	120	ARG	3.8
52	2u	10	ARG	3.8
52	2u	22	ARG	3.8
32	1a	1358	U	3.8
29	27	1	MET	3.8
40	2i	122	ALA	3.8
14	2S	31	SER	3.8
45	2n	8	GLU	3.8
41	1j	45	ARG	3.8
11	2P	68	GLN	3.8
1	2A	2319	G	3.8
22	20	74	ARG	3.8
41	1j	44	VAL	3.8
55	2z	12	ARG	3.8
13	2R	13	HIS	3.8
44	1m	123	ALA	3.7
45	1n	57	ARG	3.7
45	1n	34	TYR	3.7
36	2e	13	ILE	3.7
44	1m	2	ALA	3.7
12	2Q	39	PRO	3.7
40	2i	121	ARG	3.7
7	2H	159	GLU	3.7
47	1p	1	MET	3.7
40	2i	64	THR	3.7
45	2n	37	PHE	3.7
45	1n	15	LYS	3.7
52	1u	16	GLY	3.7
1	2A	2145	C	3.7
41	2j	45	ARG	3.7
47	1p	5	ARG	3.7
41	2j	63	PHE	3.7
45	2n	58	LYS	3.7
32	2a	975	A	3.7
47	1p	15	PRO	3.7
51	1t	71	THR	3.6
51	1t	73	HIS	3.6
40	2i	7	THR	3.6
47	1p	17	TYR	3.6
45	2n	6	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
38	2g	78	ARG	3.6
45	2n	31	ARG	3.6
1	2A	2146	C	3.6
8	2I	12	LEU	3.6
39	2h	133	LEU	3.6
51	1t	22	ARG	3.6
13	2R	51	LEU	3.6
32	1a	1354	C	3.6
44	1m	105	THR	3.6
52	2u	5	ASP	3.6
44	1m	102	ARG	3.6
44	2m	121	LYS	3.6
9	2N	69	GLN	3.6
32	2a	965	A	3.6
40	1i	65	VAL	3.6
29	27	46	VAL	3.6
32	1a	1359	C	3.6
51	2t	74	LYS	3.6
45	1n	13	THR	3.6
39	1h	5	PRO	3.5
29	17	47	ARG	3.5
41	2j	56	HIS	3.5
45	2n	36	PHE	3.5
39	2h	12	ARG	3.5
45	1n	37	PHE	3.5
32	2a	1257	U	3.5
41	2j	40	LEU	3.5
51	2t	83	ARG	3.5
4	2E	126	PRO	3.5
22	20	42	GLY	3.5
32	1a	1353	G	3.5
52	2u	9	ARG	3.5
36	2e	81	GLU	3.5
47	1p	36	ILE	3.5
39	2h	91	ARG	3.5
13	2R	14	SER	3.5
35	1d	5	ILE	3.5
23	21	22	GLY	3.5
40	1i	107	ARG	3.5
5	2F	49	ALA	3.5
32	2a	1511	G	3.5
32	1a	1363(A)	A	3.5

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Mol	Chain	Res	Type	RSRZ
41	1j	61	GLU	3.5
48	2q	24	GLU	3.5
44	2m	98	VAL	3.5
12	2Q	38	GLU	3.4
47	1p	65	GLN	3.4
31	29	16	VAL	3.4
32	2a	1364	U	3.4
32	1a	378	G	3.4
40	2i	15	ALA	3.4
13	2R	9	LYS	3.4
32	1a	1362	C	3.4
36	2e	22	GLY	3.4
44	2m	119	GLY	3.4
38	2g	32	ARG	3.4
13	2R	70	LEU	3.4
3	2D	217	ARG	3.4
45	1n	56	VAL	3.4
32	2a	1492	A	3.4
47	1p	68	ASP	3.4
50	2s	79	THR	3.4
51	1t	72	LEU	3.4
3	2D	37	LEU	3.4
32	1a	1529	G	3.4
39	1h	2	LEU	3.4
36	1e	25	ARG	3.4
33	2b	132	LYS	3.4
38	2g	4	ARG	3.4
40	2i	10	ARG	3.4
45	1n	29	ARG	3.4
4	2E	158	GLY	3.4
32	1a	1361	G	3.4
45	1n	39	LEU	3.4
32	2a	262	A	3.4
22	20	53	MET	3.4
44	2m	97	PRO	3.4
51	2t	13	LEU	3.4
32	2a	1353	G	3.4
40	2i	70	LYS	3.4
44	1m	122	LYS	3.4
47	1p	25	ARG	3.4
34	1c	153	VAL	3.4
39	2h	94	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
35	1d	120	LEU	3.3
1	2A	2144	U	3.3
3	2D	276	LYS	3.3
19	2X	28	PHE	3.3
13	2R	21	TYR	3.3
35	1d	23	GLY	3.3
34	1c	154	SER	3.3
48	2q	29	HIS	3.3
39	2h	92	ARG	3.3
44	2m	108	ARG	3.3
41	1j	53	PRO	3.3
9	2N	78	TYR	3.3
13	2R	20	LEU	3.3
44	2m	94	ARG	3.3
55	1z	16	ARG	3.3
9	2N	84	LYS	3.3
32	1a	1352	C	3.3
41	1j	54	PHE	3.3
4	2E	125	GLY	3.3
22	20	75	LEU	3.3
22	20	41	ARG	3.2
36	1e	24	ARG	3.2
32	1a	1355	G	3.2
32	1a	1370	G	3.2
34	2c	160	ALA	3.2
40	1i	106	ALA	3.2
31	29	15	LYS	3.2
43	2l	7	ILE	3.2
35	1d	4	TYR	3.2
43	2l	64	TYR	3.2
32	2a	1236	A	3.2
47	1p	42	ARG	3.2
33	2b	202	PRO	3.2
48	1q	28	PRO	3.2
45	1n	31	ARG	3.2
51	1t	13	LEU	3.2
45	2n	17	LYS	3.2
4	2E	10	GLY	3.2
32	2a	964	A	3.2
32	2a	969	A	3.2
7	2H	107	VAL	3.2
40	2i	37	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
12	2Q	17	LEU	3.2
15	2T	50	ILE	3.2
41	2j	53	PRO	3.2
52	2u	12	LYS	3.2
51	1t	19	SER	3.2
52	1u	22	ARG	3.2
3	2D	215	LEU	3.2
9	2N	43	THR	3.2
13	2R	1	MET	3.2
30	28	59	LYS	3.2
40	2i	112	LYS	3.2
20	2Y	45	VAL	3.2
23	21	98	LEU	3.2
32	2a	977	A	3.2
32	2a	1363(A)	A	3.2
48	2q	71	PHE	3.2
48	1q	29	HIS	3.2
7	2H	103	LEU	3.2
51	1t	20	LEU	3.2
45	1n	16	PHE	3.2
40	2i	71	SER	3.2
39	2h	3	THR	3.2
43	2l	15	ARG	3.1
35	1d	137	SER	3.1
51	2t	30	LYS	3.1
39	2h	86	ILE	3.1
25	23	17	LYS	3.1
52	2u	15	ARG	3.1
4	2E	150	VAL	3.1
45	1n	41	ARG	3.1
47	2p	7	ALA	3.1
1	2A	1379	A	3.1
22	20	46	LYS	3.1
32	1a	971	G	3.1
32	2a	951	G	3.1
52	1u	13	ILE	3.1
4	2E	116	VAL	3.1
41	2j	54	PHE	3.1
45	2n	60	SER	3.1
14	2S	92	TYR	3.1
13	2R	8	ARG	3.1
20	2Y	2	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
23	21	21	ARG	3.1
32	2a	1050	G	3.1
47	1p	16	HIS	3.1
51	2t	75	ASN	3.1
39	2h	84	ARG	3.1
6	2G	161	THR	3.1
47	1p	39	TYR	3.1
32	2a	1286	A	3.1
29	27	47	ARG	3.1
39	2h	131	GLY	3.1
40	2i	108	VAL	3.1
47	1p	35	LYS	3.1
43	2l	10	LEU	3.1
38	2g	83	ALA	3.0
40	2i	72	GLY	3.0
51	1t	9	ASN	3.0
6	2G	39	ILE	3.0
31	29	3	VAL	3.0
32	2a	1223	C	3.0
41	1j	66	ARG	3.0
3	1D	275	LYS	3.0
51	1t	14	LYS	3.0
34	1c	193	TYR	3.0
23	21	68	PRO	3.0
48	2q	39	SER	3.0
22	20	45	PHE	3.0
32	2a	1250	A	3.0
40	1i	124	GLN	3.0
45	1n	30	ALA	3.0
51	1t	17	ARG	3.0
32	2a	983	A	3.0
16	2U	18	LEU	3.0
47	1p	60	LEU	3.0
45	1n	36	PHE	3.0
50	2s	38	SER	3.0
3	2D	256	GLY	3.0
51	2t	14	LYS	3.0
44	2m	99	ARG	3.0
45	2n	10	ALA	3.0
50	2s	35	SER	3.0
32	2a	112	G	3.0
32	2a	963	G	3.0

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Mol	Chain	Res	Type	RSRZ
51	2t	66	ALA	3.0
14	2S	32	LEU	3.0
35	1d	118	ARG	3.0
1	2A	2690	C	3.0
39	2h	85	ARG	3.0
43	2l	13	LYS	3.0
41	2j	6	ILE	3.0
47	1p	8	ARG	3.0
45	1n	24	CYS	3.0
22	20	68	GLU	3.0
38	1g	80	VAL	2.9
3	2D	38	LYS	2.9
9	2N	83	LYS	2.9
45	2n	38	GLY	2.9
13	2R	10	LEU	2.9
45	1n	25	VAL	2.9
32	1a	377	G	2.9
23	11	2	SER	2.9
13	2R	18	LEU	2.9
20	2Y	35	TYR	2.9
32	1a	969	A	2.9
44	2m	96	LEU	2.9
36	1e	82	VAL	2.9
32	2a	978	A	2.9
13	2R	7	GLY	2.9
47	1p	33	ILE	2.9
22	20	80	HIS	2.9
51	2t	73	HIS	2.9
11	2P	51	PHE	2.9
32	1a	1233	G	2.9
1	1A	2132	U	2.9
9	2N	44	PRO	2.9
43	1l	5	PRO	2.9
4	2E	157	ALA	2.9
30	28	64	TYR	2.9
41	1j	55	LYS	2.9
47	1p	59	TRP	2.9
34	1c	155	GLY	2.9
30	28	16	ILE	2.9
44	2m	78	ILE	2.9
32	2a	1221	G	2.9
44	1m	87	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	2A	1555	G	2.9
32	2a	1235	U	2.9
20	2Y	7	VAL	2.9
41	2j	98	ILE	2.9
48	2q	42	TYR	2.9
13	2R	43	GLU	2.9
50	2s	14	HIS	2.9
52	1u	15	ARG	2.9
51	2t	21	LYS	2.9
32	2a	1289	A	2.9
45	2n	23	ARG	2.9
31	19	34	GLN	2.8
32	2a	232	G	2.8
9	2N	76	SER	2.8
29	17	1	MET	2.8
38	1g	78	ARG	2.8
44	1m	104	ARG	2.8
48	1q	27	PHE	2.8
30	28	15	LYS	2.8
32	2a	982	U	2.8
6	2G	160	VAL	2.8
50	2s	41	VAL	2.8
13	2R	22	ARG	2.8
47	1p	31	LYS	2.8
47	1p	80	PHE	2.8
36	1e	22	GLY	2.8
47	1p	28	ARG	2.8
51	2t	84	LEU	2.8
55	2z	15	PRO	2.8
34	2c	206	GLU	2.8
17	2V	74	LYS	2.8
48	2q	33	GLY	2.8
22	20	69	PHE	2.8
1	1A	1094	U	2.8
3	2D	35	LYS	2.8
38	2g	10	ARG	2.8
13	2R	6	SER	2.8
35	1d	179	GLU	2.8
6	2G	133	LEU	2.8
44	1m	107	ALA	2.8
25	23	19	GLN	2.8
39	2h	95	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
34	1c	4	LYS	2.8
48	2q	69	LYS	2.8
11	2P	35	HIS	2.8
35	1d	102	ASP	2.8
38	2g	81	GLY	2.8
23	21	14	VAL	2.8
20	2Y	34	LYS	2.8
22	20	72	ARG	2.8
24	22	2	LYS	2.8
39	2h	132	GLU	2.8
47	2p	26	ARG	2.8
30	18	7	HIS	2.8
32	1a	968	A	2.8
41	1j	43	ARG	2.8
41	2j	65	LEU	2.8
23	11	36	GLY	2.8
11	1P	15	ARG	2.8
51	1t	24	LEU	2.8
45	1n	10	ALA	2.8
22	20	44	ARG	2.8
1	2A	2713	A	2.7
3	2D	247	ALA	2.7
13	2R	47	PHE	2.7
30	28	24	ALA	2.7
32	1a	1286	A	2.7
35	1d	73	ARG	2.7
38	1g	84	ASN	2.7
43	2l	19	ARG	2.7
32	2a	1116	C	2.7
22	20	11	ARG	2.7
35	1d	6	GLY	2.7
43	2l	11	VAL	2.7
35	2d	49	ARG	2.7
38	2g	16	LEU	2.7
43	2l	28	LYS	2.7
16	1U	4	ALA	2.7
20	2Y	59	GLY	2.7
34	1c	152	ILE	2.7
11	2P	72	PRO	2.7
44	1m	97	PRO	2.7
32	1a	974	A	2.7
1	2A	2128	C	2.7

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Mol	Chain	Res	Type	RSRZ
38	2g	85	TYR	2.7
9	2N	23	LEU	2.7
11	2P	59	LEU	2.7
25	23	53	LEU	2.7
47	1p	67	THR	2.7
32	2a	238	G	2.7
43	1l	26	ALA	2.7
11	2P	74	GLU	2.7
13	2R	40	LYS	2.7
14	2S	3	ARG	2.7
39	2h	35	ILE	2.7
1	1A	2145	C	2.7
3	1D	37	LEU	2.7
3	2D	53	PHE	2.7
52	2u	8	THR	2.7
3	2D	221	VAL	2.7
3	2D	275	LYS	2.7
23	21	62	VAL	2.7
29	27	23	ARG	2.7
40	2i	83	ARG	2.7
33	2b	135	GLN	2.7
12	2Q	104	PHE	2.7
45	1n	38	GLY	2.7
13	2R	25	ALA	2.7
40	2i	111	ARG	2.7
3	2D	257	LEU	2.7
30	28	63	PRO	2.7
32	2a	1531	A	2.7
47	2p	27	LYS	2.7
30	28	22	VAL	2.7
44	2m	111	LYS	2.7
39	2h	87	SER	2.7
39	1h	89	PRO	2.7
45	1n	51	GLY	2.7
8	2I	13	GLY	2.7
9	2N	8	GLN	2.7
23	21	28	GLY	2.7
36	2e	133	TYR	2.6
39	2h	83	ILE	2.7
13	2R	44	LEU	2.6
48	2q	68	ARG	2.6
32	2a	1225	A	2.6

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Mol	Chain	Res	Type	RSRZ
34	1c	196	LEU	2.6
43	2l	101	VAL	2.6
45	2n	9	LYS	2.6
51	2t	29	LYS	2.6
3	2D	61	LEU	2.6
2	2B	88	C	2.6
31	29	1	MET	2.6
35	1d	62	GLN	2.6
44	2m	109	THR	2.6
45	2n	19	ARG	2.6
48	1q	36	ILE	2.6
16	1U	9	VAL	2.6
32	1a	1369	C	2.6
39	1h	92	ARG	2.6
41	2j	43	ARG	2.6
47	2p	29	ASP	2.6
12	2Q	37	LEU	2.6
27	25	2	ALA	2.6
30	18	2	PRO	2.6
32	1a	1349	A	2.6
32	1a	1447	A	2.6
32	2a	1349	A	2.6
1	2A	2143	C	2.6
31	19	12	ASP	2.6
4	1E	157	ALA	2.6
31	29	2	LYS	2.6
3	2D	52	ARG	2.6
34	1c	10	PHE	2.6
32	2a	941	G	2.6
41	2j	52	GLY	2.6
47	2p	19	ILE	2.6
13	2R	11	ASN	2.6
51	1t	80	ARG	2.6
23	21	29	GLY	2.6
32	2a	972	C	2.6
45	1n	20	ALA	2.6
9	2N	73	THR	2.6
32	1a	112	G	2.6
17	2V	71	LEU	2.6
34	2c	6	HIS	2.6
4	2E	114	ALA	2.6
50	2s	12	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
51	1t	69	GLY	2.6
22	20	58	THR	2.6
52	2u	23	PRO	2.6
30	28	58	ILE	2.6
32	1a	311	C	2.6
34	2c	162	GLN	2.6
35	1d	80	GLU	2.6
15	2T	99	LEU	2.6
3	2D	39	LYS	2.5
13	2R	24	GLN	2.5
34	2c	163	ALA	2.5
2	2B	59	A	2.5
1	2A	2035	G	2.5
48	1q	23	VAL	2.5
48	2q	12	SER	2.5
44	2m	87	TYR	2.5
11	2P	20	GLY	2.5
16	2U	9	VAL	2.5
20	2Y	3	VAL	2.5
1	2A	2724	C	2.5
32	1a	1287	A	2.5
32	2a	263	A	2.5
36	2e	31	LEU	2.5
15	2T	48	ILE	2.5
52	2u	3	LYS	2.5
3	2D	233	HIS	2.5
9	2N	74	ARG	2.5
35	1d	3	ARG	2.5
50	2s	36	ARG	2.5
52	2u	24	ARG	2.5
50	2s	82	GLY	2.5
6	2G	139	LEU	2.5
31	19	13	LYS	2.5
45	2n	4	LYS	2.5
39	2h	134	ILE	2.5
48	2q	65	ILE	2.5
45	2n	12	ARG	2.5
43	1l	16	GLU	2.5
4	1E	146	THR	2.5
48	2q	10	VAL	2.5
19	2X	33	LYS	2.5
43	2l	27	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
52	1u	24	ARG	2.5
20	2Y	62	GLU	2.5
22	20	54	GLY	2.5
40	2i	29	ASN	2.5
51	2t	26	ASN	2.5
1	2A	2159	G	2.5
32	2a	823	G	2.5
43	1l	64	TYR	2.5
38	2g	84	ASN	2.5
36	2e	89	ILE	2.5
17	2V	82	ARG	2.5
32	1a	1508	G	2.5
30	18	65	GLU	2.5
30	28	29	LYS	2.5
32	2a	1249	C	2.5
11	1P	34	GLY	2.5
11	2P	71	VAL	2.5
30	28	14	VAL	2.5
31	19	25	VAL	2.5
1	1A	2141	G	2.5
9	2N	70	LYS	2.5
39	1h	88	LYS	2.5
51	1t	29	LYS	2.5
6	2G	35	GLU	2.5
40	1i	15	ALA	2.5
41	1j	52	GLY	2.5
32	1a	1531	A	2.5
5	2F	64	ILE	2.5
45	2n	21	TYR	2.5
47	1p	24	ALA	2.5
32	2a	970	C	2.4
11	2P	109	GLY	2.4
29	27	14	LYS	2.4
32	2a	968	A	2.4
47	1p	9	PHE	2.4
40	2i	73	GLN	2.4
25	23	26	LEU	2.4
38	1g	35	LYS	2.4
50	2s	34	TRP	2.4
34	2c	158	GLY	2.4
32	1a	1188	A	2.4
47	2p	28	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
51	2t	79	ARG	2.4
31	19	28	GLU	2.4
41	1j	56	HIS	2.4
48	1q	40	LYS	2.4
24	22	24	LEU	2.4
43	2l	32	PHE	2.4
51	2t	76	ALA	2.4
1	1A	2697	G	2.4
32	2a	121	C	2.4
31	29	13	LYS	2.4
34	1c	5	ILE	2.4
47	1p	22	THR	2.4
39	1h	10	LEU	2.4
39	2h	9	MET	2.4
20	2Y	69	ALA	2.4
11	2P	75	ILE	2.4
39	2h	88	LYS	2.4
44	1m	96	LEU	2.4
2	2B	89	G	2.4
4	2E	134	ILE	2.4
48	1q	24	GLU	2.4
3	2D	235	GLY	2.4
41	1j	10	GLY	2.4
32	2a	1357	A	2.4
47	1p	32	TYR	2.4
45	2n	57	ARG	2.4
31	29	25	VAL	2.4
36	1e	128	PRO	2.4
36	2e	19	MET	2.4
36	2e	123	LEU	2.4
44	2m	95	GLY	2.4
47	1p	2	VAL	2.4
43	1l	28	LYS	2.4
4	2E	137	HIS	2.4
32	2a	950	U	2.4
52	1u	10	ARG	2.4
8	2I	35	LEU	2.4
32	2a	1092	A	2.4
33	2b	101	MET	2.4
34	1c	151	VAL	2.4
40	1i	11	LYS	2.4
40	1i	108	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
50	2s	71	LEU	2.4
52	1u	11	GLY	2.4
34	1c	201	TYR	2.4
55	2z	16	ARG	2.4
32	1a	1364	U	2.4
6	2G	159	VAL	2.4
16	1U	8	VAL	2.4
32	1a	1363	C	2.4
40	1i	70	LYS	2.4
19	2X	85	PRO	2.4
45	1n	14	PRO	2.4
41	2j	61	GLU	2.4
39	2h	25	ASP	2.4
13	2R	4	LEU	2.4
35	1d	110	PHE	2.4
39	1h	90	GLY	2.4
32	2a	1234	C	2.4
32	2a	327	A	2.4
46	2o	47	LYS	2.4
30	18	23	VAL	2.4
23	21	61	ARG	2.4
32	1a	1511	G	2.4
52	2u	7	ARG	2.4
1	1A	34	C	2.4
31	29	24	TYR	2.4
32	2a	879	C	2.4
14	2S	5	THR	2.4
43	1l	27	LEU	2.4
22	20	77	ARG	2.3
32	2a	1525	G	2.3
23	21	34	THR	2.3
23	21	41	ARG	2.3
3	1D	219	PRO	2.3
4	2E	160	TYR	2.3
14	2S	91	PRO	2.3
33	2b	130	ARG	2.3
34	2c	188	LEU	2.3
39	1h	112	LEU	2.3
45	1n	19	ARG	2.3
12	2Q	18	LYS	2.3
32	2a	1222	G	2.3
34	2c	155	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
36	2e	90	VAL	2.3
43	1l	6	THR	2.3
6	2G	136	ARG	2.3
22	20	79	VAL	2.3
35	2d	198	VAL	2.3
7	2H	145	ALA	2.3
41	2j	96	ILE	2.3
50	1s	71	LEU	2.3
53	1v	21	C	2.3
32	1a	1532	U	2.3
32	2a	1285	A	2.3
22	20	71	ASP	2.3
4	1E	152	LYS	2.3
9	2N	116	LEU	2.3
40	2i	13	ALA	2.3
52	1u	12	LYS	2.3
32	2a	1369	C	2.3
32	1a	306	G	2.3
1	2A	2712(A)	A	2.3
3	1D	253	GLN	2.3
13	2R	26	LYS	2.3
35	1d	101	LEU	2.3
3	2D	34	VAL	2.3
35	1d	112	VAL	2.3
1	1A	1093	G	2.3
1	2A	2585	U	2.3
30	28	7	HIS	2.3
50	2s	15	LEU	2.3
51	2t	72	LEU	2.3
32	2a	949	A	2.3
30	18	56	GLU	2.3
45	1n	7	ILE	2.3
14	2S	13	ARG	2.3
9	2N	109	LYS	2.3
32	2a	1526	G	2.3
47	1p	30	GLY	2.3
48	2q	66	SER	2.3
4	2E	136	ARG	2.3
22	20	38	VAL	2.3
34	2c	10	PHE	2.3
4	2E	192	ASN	2.3
32	2a	723	U	2.3

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Mol	Chain	Res	Type	RSRZ
14	2S	9	ARG	2.3
32	1a	1343	G	2.3
32	1a	1526	G	2.3
32	2a	1186	G	2.3
32	2a	1368	G	2.3
34	1c	12	LEU	2.3
35	1d	157	LEU	2.3
40	1i	47	LEU	2.3
45	1n	26	ARG	2.3
9	2N	75	TYR	2.3
14	2S	34	HIS	2.3
16	2U	16	LYS	2.3
23	21	4	VAL	2.3
35	1d	8	VAL	2.3
13	2R	17	ARG	2.3
1	1A	1099	G	2.2
23	21	16	ASN	2.2
11	2P	70	GLN	2.2
26	24	54	GLY	2.2
30	28	61	LEU	2.2
1	2A	2133	G	2.2
32	2a	1373	G	2.2
6	2G	102	PHE	2.2
43	2l	61	THR	2.2
11	2P	34	GLY	2.2
11	2P	44	GLY	2.2
32	1a	328	C	2.2
3	2D	252	TRP	2.2
11	2P	79	ARG	2.2
45	1n	12	ARG	2.2
23	11	98	LEU	2.2
42	2k	123	LYS	2.2
39	1h	3	THR	2.2
43	2l	6	THR	2.2
30	28	10	ALA	2.2
48	1q	26	GLN	2.2
52	2u	11	GLY	2.2
1	1A	1638	C	2.2
22	20	9	SER	2.2
34	2c	154	SER	2.2
22	20	78	TYR	2.2
32	2a	813	U	2.2

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Mol	Chain	Res	Type	RSRZ
1	2A	2334	G	2.2
29	27	18	PHE	2.2
32	1a	948	C	2.2
32	2a	328	C	2.2
3	2D	238	GLY	2.2
45	2n	15	LYS	2.2
47	2p	12	LYS	2.2
1	1A	1026	U	2.2
3	2D	5	LYS	2.2
36	1e	13	ILE	2.2
39	1h	137	VAL	2.2
40	2i	11	LYS	2.2
40	2i	63	ILE	2.2
1	2A	1347	G	2.2
32	2a	984	C	2.2
32	2a	1220	G	2.2
32	2a	1354	C	2.2
43	2l	31	PRO	2.2
44	1m	121	LYS	2.2
45	2n	50	LYS	2.2
14	2S	12	PHE	2.2
32	1a	1001(A)	G	2.2
32	2a	947	G	2.2
25	23	51	ALA	2.2
34	1c	168	ALA	2.2
47	2p	64	ALA	2.2
22	20	40	GLN	2.2
30	18	5	LYS	2.2
1	1A	1092	C	2.2
1	2A	1656	C	2.2
32	2a	824	C	2.2
47	2p	4	ILE	2.2
1	2A	1125	G	2.2
4	1E	153	GLY	2.2
32	2a	1064	G	2.2
51	2t	22	ARG	2.2
32	2a	325	A	2.2
32	2a	766	A	2.2
4	2E	141	ILE	2.2
20	1Y	1	MET	2.2
36	1e	122	GLU	2.2
22	20	73	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
36	2e	124	GLY	2.2
4	1E	155	LYS	2.2
41	2j	51	ARG	2.2
18	2W	86	LEU	2.2
43	1l	98	TYR	2.2
32	1a	323	U	2.2
1	2A	2147	G	2.2
32	1a	111	G	2.2
51	2t	18	GLN	2.2
5	2F	78	ILE	2.2
22	20	23	VAL	2.2
23	21	33	LYS	2.2
32	2a	1066	C	2.1
36	2e	92	LYS	2.1
48	1q	34	LYS	2.1
32	2a	1233	G	2.1
3	2D	254	THR	2.1
35	1d	11	LEU	2.1
40	2i	79	LEU	2.1
5	2F	90	PHE	2.1
3	2D	212	SER	2.1
3	2D	249	PRO	2.1
3	2D	273	ARG	2.1
16	1U	13	LYS	2.1
47	2p	5	ARG	2.1
39	2h	54	ASP	2.1
49	1r	78	LEU	2.1
3	2D	153	ALA	2.1
4	2E	135	HIS	2.1
29	27	15	THR	2.1
40	1i	37	PHE	2.1
51	2t	78	ALA	2.1
25	23	10	LYS	2.1
30	28	46	ARG	2.1
32	2a	331	G	2.1
35	2d	209	ARG	2.1
31	29	17	ILE	2.1
40	2i	67	GLY	2.1
47	1p	66	PRO	2.1
1	1A	1065	U	2.1
1	1A	2138	C	2.1
22	20	21	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
45	2n	47	LEU	2.1
9	2N	72	TYR	2.1
13	2R	12	ARG	2.1
30	28	30	ARG	2.1
31	19	8	LYS	2.1
41	1j	11	PHE	2.1
47	2p	8	ARG	2.1
36	1e	100	VAL	2.1
6	2G	2	PRO	2.1
20	2Y	31	LEU	2.1
32	1a	108	G	2.1
32	1a	1186	G	2.1
34	1c	26	LYS	2.1
51	1t	23	ARG	2.1
34	2c	173	VAL	2.1
4	2E	115	GLY	2.1
39	2h	89	PRO	2.1
11	2P	65	ARG	2.1
32	1a	313	A	2.1
32	1a	1528	U	2.1
19	1X	56	THR	2.1
32	2a	1226	C	2.1
35	1d	2	GLY	2.1
40	2i	118	LYS	2.1
4	2E	191	PRO	2.1
34	1c	169	ALA	2.1
3	2D	49	ILE	2.1
26	24	40	HIS	2.1
32	1a	977	A	2.1
32	2a	974	A	2.1
19	2X	68	ARG	2.1
23	21	25	LYS	2.1
32	2a	1231	G	2.1
44	1m	103	THR	2.1
4	1E	116	VAL	2.1
5	2F	82	ILE	2.1
14	2S	93	LYS	2.1
15	2T	63	VAL	2.1
31	29	23	VAL	2.1
33	2b	214	ILE	2.1
36	1e	92	LYS	2.1
40	1i	75	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
43	1l	91	LYS	2.1
45	2n	44	LEU	2.1
46	2o	66	LEU	2.1
48	1q	31	LEU	2.1
48	2q	6	LEU	2.1
3	1D	254	THR	2.1
1	2A	696	G	2.1
32	1a	980	C	2.1
6	2G	37	VAL	2.1
11	2P	108	LYS	2.1
15	2T	98	LYS	2.1
22	20	39	ARG	2.1
31	29	8	LYS	2.1
6	2G	26	GLN	2.1
30	28	35	GLN	2.1
43	1l	29	GLY	2.1
1	1A	1078	U	2.1
48	2q	27	PHE	2.1
13	2R	42	LYS	2.1
45	2n	56	VAL	2.1
48	2q	25	ARG	2.1
39	1h	6	ILE	2.1
1	2A	1377	G	2.1
13	2R	111	LEU	2.1
20	2Y	6	HIS	2.1
32	1a	231	G	2.1
32	1a	973	G	2.1
32	1a	1190	G	2.1
32	2a	1343	G	2.1
47	2p	6	LEU	2.1
26	24	49	PHE	2.1
3	1D	38	LYS	2.1
32	1a	1348	U	2.1
35	1d	68	TYR	2.1
11	1P	45	LEU	2.1
14	2S	35	ILE	2.1
15	2T	102	ILE	2.1
20	2Y	61	ILE	2.1
4	2E	153	GLY	2.1
32	1a	1503	A	2.1
32	2a	1346	A	2.1
51	2t	69	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	2A	1382	G	2.0
30	18	53	PRO	2.0
40	2i	28	VAL	2.0
48	2q	9	VAL	2.0
30	18	3	LYS	2.0
13	1R	49	ASP	2.0
20	2Y	68	HIS	2.0
1	1A	2137	C	2.0
1	2A	1350	C	2.0
1	2A	2111	C	2.0
8	2I	18	VAL	2.0
13	2R	48	VAL	2.0
35	1d	148	VAL	2.0
9	2N	45	ASN	2.0
13	2R	39	PRO	2.0
28	16	10	LEU	2.0
36	1e	89	ILE	2.0
43	2l	8	ASN	2.0
32	2a	326	G	2.0
32	2a	727	G	2.0
3	2D	222	ARG	2.0
35	1d	75	PHE	2.0
26	24	51	ASP	2.0
32	1a	1513	A	2.0
3	2D	204	ILE	2.0
20	2Y	65	ALA	2.0
32	2a	1115	C	2.0
32	2a	1322	C	2.0
43	1l	7	ILE	2.0
44	2m	5	ALA	2.0
46	2o	87	ILE	2.0
4	1E	147	PRO	2.0
18	2W	104	THR	2.0
38	1g	34	GLY	2.0
32	1a	1202	G	2.0
32	2a	1371	G	2.0
33	2b	108	ILE	2.0
33	2b	215	LEU	2.0
1	1A	529	A	2.0
32	2a	815	A	2.0
35	1d	66	ARG	2.0
51	1t	15	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
6	2G	29	TRP	2.0
9	2N	114	ARG	2.0
18	2W	94	ASP	2.0
45	1n	9	LYS	2.0
3	2D	64	ILE	2.0
32	2a	769	G	2.0
5	2F	51	THR	2.0
31	29	34	GLN	2.0
32	2a	1030(B)	C	2.0
14	2S	4	LEU	2.0
38	1g	85	TYR	2.0
48	1q	35	VAL	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	4SU	2x	8	20/21	0.91	0.12	69,83,95,100	0
54	PSU	2x	55	20/21	0.91	0.13	75,83,87,87	0
1	5MU	2A	1915	21/22	0.92	0.14	64,79,83,84	0
32	5MC	2a	967	21/22	0.92	0.34	62,73,80,86	0
1	5MU	1A	1915	21/22	0.92	0.16	64,75,82,97	0
54	PSU	1x	55	20/21	0.92	0.16	56,67,76,82	0
43	0TD	2l	92	10/11	0.93	0.21	63,69,73,80	0
32	M2G	2a	966	25/26	0.93	0.29	64,70,82,85	0
54	5MU	2x	54	21/22	0.93	0.16	73,80,87,94	0
32	2MG	2a	1207	24/25	0.93	0.17	69,82,87,90	0
43	0TD	1l	92	10/11	0.94	0.15	54,61,67,68	0
54	4SU	1x	8	20/21	0.94	0.18	65,70,77,81	0
32	4OC	2a	1402	22/23	0.94	0.22	61,67,72,77	0
1	PSU	1A	1917	20/21	0.94	0.16	52,67,74,75	0
32	PSU	1a	516	20/21	0.94	0.15	68,73,77,78	0
54	5MC	2x	32	21/22	0.94	0.27	65,74,78,80	0
1	4OC	2A	1920	21/23	0.94	0.20	61,68,73,80	0
32	2MG	1a	1207	24/25	0.94	0.18	65,71,79,86	0
32	MA6	2a	1518	24/25	0.95	0.25	56,64,68,70	0
1	PSU	1A	1911	20/21	0.95	0.18	58,66,67,69	0
1	PSU	2A	1911	20/21	0.95	0.15	54,67,70,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	PSU	2a	516	20/21	0.95	0.12	72,79,81,87	0
32	7MG	2a	527	24/25	0.95	0.17	63,67,75,77	0
32	5MC	2a	1404	21/22	0.95	0.26	58,65,70,73	0
32	M2G	1a	966	25/26	0.96	0.35	55,63,68,73	0
32	5MC	1a	967	21/22	0.96	0.37	59,67,72,76	0
54	5MU	1x	54	21/22	0.96	0.15	64,67,72,78	0
32	7MG	1a	527	24/25	0.96	0.18	51,57,66,73	0
32	4OC	1a	1402	22/23	0.96	0.20	58,61,65,74	0
32	5MC	2a	1400	21/22	0.96	0.25	63,66,71,77	0
32	5MC	1a	1404	21/22	0.96	0.22	37,56,62,65	0
1	PSU	2A	1917	20/21	0.96	0.14	67,75,82,84	0
32	MA6	1a	1518	24/25	0.96	0.28	46,55,61,63	0
1	5MC	2A	1942	21/22	0.96	0.18	52,63,73,76	0
1	5MC	2A	1962	21/22	0.96	0.21	46,59,63,72	0
1	OMG	2A	2251	24/25	0.96	0.28	44,49,54,59	0
1	2MA	2A	2503	23/24	0.96	0.23	37,43,51,56	0
1	PSU	2A	2605	20/21	0.96	0.28	41,48,51,52	0
1	5MU	2A	1939	21/22	0.97	0.25	41,54,59,64	0
1	2MU	1A	2552	21/23	0.97	0.22	40,43,50,51	0
1	PSU	1A	2605	20/21	0.97	0.23	35,40,44,48	0
54	5MC	1x	32	21/22	0.97	0.23	50,61,69,75	0
32	5MC	2a	1407	21/22	0.97	0.20	60,64,68,71	0
32	UR3	2a	1498	21/22	0.97	0.23	53,59,64,72	0
32	5MC	1a	1400	21/22	0.97	0.25	57,61,66,70	0
32	MA6	2a	1519	24/25	0.97	0.30	54,65,68,69	0
1	4OC	1A	1920	21/23	0.97	0.23	34,57,65,66	0
1	5MC	1A	1942	21/22	0.97	0.21	47,52,59,64	0
32	5MC	1a	1407	21/22	0.97	0.23	44,53,61,61	0
1	5MC	1A	1962	21/22	0.97	0.21	39,51,59,68	0
32	MA6	1a	1519	24/25	0.97	0.29	48,56,60,69	0
32	UR3	1a	1498	21/22	0.98	0.21	41,50,53,56	0
1	2MU	2A	2552	21/23	0.98	0.20	43,49,56,59	0
1	2MA	1A	2503	23/24	0.98	0.26	22,35,40,45	0
1	5MU	1A	1939	21/22	0.98	0.20	37,43,47,52	0
1	OMG	1A	2251	24/25	0.98	0.20	27,39,44,45	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, 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
56	MG	1A	3338	1/1	0.42	0.29	70,70,70,70	0
56	MG	2A	3366	1/1	0.50	0.18	64,64,64,64	0
56	MG	1A	3925	1/1	0.51	0.67	82,82,82,82	0
56	MG	1A	3954	1/1	0.55	0.15	39,39,39,39	0
56	MG	1A	3819	1/1	0.55	0.23	52,52,52,52	0
56	MG	1A	3923	1/1	0.56	0.12	72,72,72,72	0
56	MG	2A	3359	1/1	0.58	0.19	67,67,67,67	0
56	MG	1A	3390	1/1	0.58	0.80	56,56,56,56	0
56	MG	1A	3744	1/1	0.60	0.17	27,27,27,27	0
56	MG	1A	4041	1/1	0.61	0.40	69,69,69,69	0
56	MG	2A	3163	1/1	0.63	0.25	63,63,63,63	0
56	MG	2A	3733	1/1	0.63	0.08	76,76,76,76	0
56	MG	1A	3936	1/1	0.64	0.88	97,97,97,97	0
56	MG	2A	3279	1/1	0.64	0.38	54,54,54,54	0
56	MG	2A	3307	1/1	0.64	0.14	61,61,61,61	0
56	MG	2a	3075	1/1	0.64	0.18	56,56,56,56	0
56	MG	1a	1808	1/1	0.65	0.07	82,82,82,82	0
56	MG	1A	3313	1/1	0.66	0.48	53,53,53,53	0
56	MG	1a	1609	1/1	0.66	0.19	59,59,59,59	0
56	MG	1a	1712	1/1	0.66	0.40	64,64,64,64	0
56	MG	1a	1733	1/1	0.66	0.17	81,81,81,81	0
56	MG	2A	3615	1/1	0.66	0.14	52,52,52,52	0
56	MG	1A	3937	1/1	0.66	0.26	81,81,81,81	0
56	MG	1A	3715	1/1	0.66	0.18	51,51,51,51	0
56	MG	1a	1679	1/1	0.68	0.19	78,78,78,78	0
56	MG	1A	3554	1/1	0.68	0.17	51,51,51,51	0
56	MG	1x	110	1/1	0.68	0.27	76,76,76,76	0
56	MG	2A	3069	1/1	0.68	0.63	63,63,63,63	0
56	MG	1A	3939	1/1	0.69	0.16	64,64,64,64	0
56	MG	2A	3209	1/1	0.69	1.02	64,64,64,64	0
56	MG	2A	3277	1/1	0.69	1.46	74,74,74,74	0
56	MG	2A	3042	1/1	0.69	0.15	78,78,78,78	0
56	MG	2A	3786	1/1	0.69	0.21	79,79,79,79	0
56	MG	2a	3022	1/1	0.69	1.25	60,60,60,60	0
56	MG	1A	3438	1/1	0.69	0.25	54,54,54,54	0
56	MG	2A	3184	1/1	0.70	1.06	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3599	1/1	0.70	0.15	64,64,64,64	0
56	MG	1A	3445	1/1	0.70	0.36	57,57,57,57	0
56	MG	2a	3109	1/1	0.70	0.59	60,60,60,60	0
56	MG	2A	3658	1/1	0.71	0.17	54,54,54,54	0
56	MG	2A	3709	1/1	0.71	0.19	69,69,69,69	0
56	MG	1A	4015	1/1	0.71	0.11	61,61,61,61	0
56	MG	2A	3309	1/1	0.71	0.23	66,66,66,66	0
56	MG	1A	3750	1/1	0.71	0.18	54,54,54,54	0
56	MG	1B	225	1/1	0.71	0.16	62,62,62,62	0
56	MG	2A	3170	1/1	0.71	0.20	66,66,66,66	0
56	MG	1a	1816	1/1	0.72	0.11	76,76,76,76	0
56	MG	2A	3445	1/1	0.72	0.13	58,58,58,58	0
56	MG	2A	3678	1/1	0.72	0.21	63,63,63,63	0
56	MG	2a	3144	1/1	0.72	0.09	58,58,58,58	0
56	MG	2a	3209	1/1	0.72	0.37	76,76,76,76	0
56	MG	2A	3080	1/1	0.73	0.86	53,53,53,53	0
56	MG	2a	3077	1/1	0.73	0.09	70,70,70,70	0
56	MG	2A	3263	1/1	0.73	0.42	58,58,58,58	0
56	MG	2a	3114	1/1	0.73	0.15	60,60,60,60	0
56	MG	1A	3739	1/1	0.73	0.32	74,74,74,74	0
56	MG	2A	3187	1/1	0.73	0.23	58,58,58,58	0
56	MG	2A	3634	1/1	0.74	0.24	58,58,58,58	0
56	MG	1A	3309	1/1	0.74	0.28	59,59,59,59	0
56	MG	2A	3035	1/1	0.74	0.11	67,67,67,67	0
56	MG	1A	3401	1/1	0.74	0.23	48,48,48,48	0
56	MG	2A	3064	1/1	0.74	0.15	49,49,49,49	0
56	MG	2a	3124	1/1	0.74	0.13	60,60,60,60	0
56	MG	1f	202	1/1	0.74	0.17	60,60,60,60	0
56	MG	2E	304	1/1	0.74	0.17	50,50,50,50	0
56	MG	2A	3265	1/1	0.75	0.23	58,58,58,58	0
56	MG	1a	1771	1/1	0.75	0.08	70,70,70,70	0
56	MG	1s	101	1/1	0.75	0.20	61,61,61,61	0
56	MG	2a	3120	1/1	0.75	0.27	67,67,67,67	0
56	MG	1v	101	1/1	0.75	0.27	68,68,68,68	0
56	MG	1A	3962	1/1	0.75	0.50	81,81,81,81	0
56	MG	2a	3171	1/1	0.75	0.49	70,70,70,70	0
56	MG	1A	3440	1/1	0.75	0.42	48,48,48,48	0
56	MG	1A	4014	1/1	0.76	0.11	49,49,49,49	0
56	MG	2A	3022	1/1	0.76	0.41	56,56,56,56	0
56	MG	2A	3435	1/1	0.76	0.26	64,64,64,64	0
56	MG	2a	3127	1/1	0.76	0.10	71,71,71,71	0
56	MG	1A	3321	1/1	0.76	0.26	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	3716	1/1	0.76	0.45	68,68,68,68	0
56	MG	2A	3319	1/1	0.76	0.65	83,83,83,83	0
56	MG	2F	301	1/1	0.77	0.26	50,50,50,50	0
56	MG	2A	3468	1/1	0.77	0.82	59,59,59,59	0
56	MG	2a	3023	1/1	0.77	0.17	55,55,55,55	0
56	MG	2A	3599	1/1	0.77	0.14	38,38,38,38	0
56	MG	2A	3190	1/1	0.77	0.16	49,49,49,49	0
56	MG	1a	1660	1/1	0.77	1.03	63,63,63,63	0
56	MG	1A	3487	1/1	0.77	0.40	52,52,52,52	0
56	MG	2A	3332	1/1	0.77	0.73	51,51,51,51	0
56	MG	2A	3350	1/1	0.77	0.32	71,71,71,71	0
56	MG	1A	3827	1/1	0.77	0.26	75,75,75,75	0
56	MG	2A	3066	1/1	0.77	0.54	67,67,67,67	0
56	MG	2a	3155	1/1	0.77	0.23	72,72,72,72	0
56	MG	2A	3030	1/1	0.77	1.31	54,54,54,54	0
56	MG	2A	3292	1/1	0.77	0.48	66,66,66,66	0
56	MG	1A	3515	1/1	0.78	0.18	54,54,54,54	0
56	MG	1a	1691	1/1	0.78	0.29	62,62,62,62	0
56	MG	1A	3871	1/1	0.78	0.10	57,57,57,57	0
56	MG	1A	3447	1/1	0.78	0.17	50,50,50,50	0
56	MG	1x	109	1/1	0.78	0.16	60,60,60,60	0
56	MG	1A	3457	1/1	0.78	0.28	52,52,52,52	0
56	MG	2a	3006	1/1	0.78	0.10	59,59,59,59	0
56	MG	2A	3222	1/1	0.78	0.90	69,69,69,69	0
56	MG	1A	3304	1/1	0.78	0.26	62,62,62,62	0
56	MG	2A	3111	1/1	0.78	0.22	69,69,69,69	0
56	MG	1A	3330	1/1	0.79	0.26	52,52,52,52	0
56	MG	2A	3493	1/1	0.79	0.11	57,57,57,57	0
56	MG	1P	204	1/1	0.79	0.92	54,54,54,54	0
56	MG	1T	201	1/1	0.79	0.24	59,59,59,59	0
56	MG	1T	203	1/1	0.79	0.23	56,56,56,56	0
56	MG	2a	3091	1/1	0.79	0.14	61,61,61,61	0
56	MG	2A	3315	1/1	0.79	0.29	67,67,67,67	0
56	MG	1A	3996	1/1	0.79	0.17	38,38,38,38	0
56	MG	1A	3465	1/1	0.79	1.58	56,56,56,56	0
56	MG	1a	1667	1/1	0.79	0.24	82,82,82,82	0
56	MG	1A	3455	1/1	0.79	0.30	46,46,46,46	0
56	MG	2a	3136	1/1	0.79	0.10	75,75,75,75	0
56	MG	2A	3074	1/1	0.79	0.11	65,65,65,65	0
56	MG	1A	3927	1/1	0.79	0.36	65,65,65,65	0
56	MG	2A	3082	1/1	0.79	0.18	77,77,77,77	0
56	MG	2a	3185	1/1	0.79	0.23	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	3003	1/1	0.79	0.08	77,77,77,77	0
56	MG	1a	1606	1/1	0.80	0.20	69,69,69,69	0
56	MG	2A	3058	1/1	0.80	0.27	56,56,56,56	0
56	MG	2a	3020	1/1	0.80	0.25	63,63,63,63	0
56	MG	1A	3660	1/1	0.80	0.34	52,52,52,52	0
56	MG	2A	3442	1/1	0.80	0.43	63,63,63,63	0
56	MG	1f	201	1/1	0.80	0.18	53,53,53,53	0
56	MG	1A	3050	1/1	0.80	0.75	56,56,56,56	0
56	MG	1l	201	1/1	0.80	0.49	67,67,67,67	0
56	MG	1A	3857	1/1	0.80	1.54	72,72,72,72	0
56	MG	2A	3284	1/1	0.80	0.24	53,53,53,53	0
56	MG	2A	3290	1/1	0.80	0.50	54,54,54,54	0
56	MG	1A	3866	1/1	0.80	0.30	73,73,73,73	0
56	MG	1A	3199	1/1	0.80	0.92	58,58,58,58	0
56	MG	2a	3134	1/1	0.80	0.18	77,77,77,77	0
56	MG	1A	3344	1/1	0.80	0.21	40,40,40,40	0
56	MG	1A	3026	1/1	0.80	0.35	61,61,61,61	0
56	MG	10	106	1/1	0.80	0.17	63,63,63,63	0
56	MG	2A	3324	1/1	0.80	0.18	67,67,67,67	0
56	MG	1a	1793	1/1	0.80	0.13	80,80,80,80	0
56	MG	2A	3188	1/1	0.80	0.11	50,50,50,50	0
56	MG	2A	3717	1/1	0.81	0.28	73,73,73,73	0
56	MG	2A	3721	1/1	0.81	0.11	56,56,56,56	0
56	MG	1A	3942	1/1	0.81	0.11	53,53,53,53	0
56	MG	1A	3835	1/1	0.81	0.15	28,28,28,28	0
56	MG	2A	3793	1/1	0.81	0.24	55,55,55,55	0
56	MG	1A	3444	1/1	0.81	0.18	53,53,53,53	0
56	MG	1A	3335	1/1	0.81	0.14	47,47,47,47	0
56	MG	1A	3730	1/1	0.81	0.09	60,60,60,60	0
56	MG	1a	1708	1/1	0.81	0.83	63,63,63,63	0
56	MG	2a	3008	1/1	0.81	0.19	61,61,61,61	0
56	MG	2A	3352	1/1	0.81	0.26	47,47,47,47	0
56	MG	1A	3873	1/1	0.81	0.15	31,31,31,31	0
56	MG	1A	3428	1/1	0.81	0.59	62,62,62,62	0
56	MG	2A	3386	1/1	0.81	0.21	61,61,61,61	0
56	MG	2A	3237	1/1	0.81	0.23	56,56,56,56	0
56	MG	2A	3238	1/1	0.81	1.52	68,68,68,68	0
56	MG	2a	3095	1/1	0.81	0.26	70,70,70,70	0
56	MG	2a	3103	1/1	0.81	0.39	60,60,60,60	0
56	MG	2A	3247	1/1	0.81	0.17	61,61,61,61	0
56	MG	1a	1763	1/1	0.81	0.08	46,46,46,46	0
56	MG	1A	3533	1/1	0.81	0.63	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	3123	1/1	0.81	0.90	72,72,72,72	0
56	MG	2A	3562	1/1	0.81	0.20	51,51,51,51	0
56	MG	1A	3365	1/1	0.81	0.28	44,44,44,44	0
56	MG	1A	3932	1/1	0.81	0.15	50,50,50,50	0
56	MG	1A	3789	1/1	0.81	0.14	48,48,48,48	0
56	MG	2a	3142	1/1	0.81	0.27	63,63,63,63	0
56	MG	10	105	1/1	0.81	0.10	52,52,52,52	0
56	MG	1A	3591	1/1	0.81	0.09	29,29,29,29	0
56	MG	2A	3697	1/1	0.81	0.34	62,62,62,62	0
56	MG	2A	3294	1/1	0.81	0.68	55,55,55,55	0
56	MG	1A	3237	1/1	0.81	0.32	57,57,57,57	0
56	MG	2a	3214	1/1	0.81	0.38	64,64,64,64	0
56	MG	2x	102	1/1	0.81	0.97	69,69,69,69	0
56	MG	1a	1796	1/1	0.82	0.08	67,67,67,67	0
56	MG	1A	3347	1/1	0.82	0.43	45,45,45,45	0
56	MG	1A	3408	1/1	0.82	0.22	54,54,54,54	0
56	MG	2E	307	1/1	0.82	0.15	36,36,36,36	0
56	MG	2A	3127	1/1	0.82	0.15	70,70,70,70	0
56	MG	20	102	1/1	0.82	0.19	53,53,53,53	0
56	MG	1G	202	1/1	0.82	0.18	49,49,49,49	0
56	MG	1a	1669	1/1	0.82	0.23	50,50,50,50	0
56	MG	1A	3290	1/1	0.82	0.14	42,42,42,42	0
56	MG	2a	3011	1/1	0.82	1.00	60,60,60,60	0
56	MG	1A	3982	1/1	0.82	0.31	59,59,59,59	0
56	MG	2a	3021	1/1	0.82	0.36	75,75,75,75	0
56	MG	1A	3887	1/1	0.82	0.08	65,65,65,65	0
56	MG	1U	205	1/1	0.82	0.19	37,37,37,37	0
56	MG	1a	1715	1/1	0.82	0.24	55,55,55,55	0
56	MG	2A	3001	1/1	0.82	0.13	43,43,43,43	0
56	MG	2a	3090	1/1	0.82	0.71	73,73,73,73	0
56	MG	2A	3225	1/1	0.82	0.81	63,63,63,63	0
56	MG	2A	3228	1/1	0.82	0.27	49,49,49,49	0
56	MG	1a	1720	1/1	0.82	0.30	69,69,69,69	0
56	MG	1A	3899	1/1	0.82	0.12	50,50,50,50	0
56	MG	2A	3525	1/1	0.82	0.17	49,49,49,49	0
56	MG	1a	1737	1/1	0.82	0.21	56,56,56,56	0
56	MG	2A	3040	1/1	0.82	0.53	51,51,51,51	0
56	MG	1A	3292	1/1	0.82	0.64	49,49,49,49	0
56	MG	2A	3268	1/1	0.82	0.16	57,57,57,57	0
56	MG	1a	1766	1/1	0.82	0.17	83,83,83,83	0
56	MG	1a	1770	1/1	0.82	0.18	55,55,55,55	0
56	MG	2A	3065	1/1	0.82	0.29	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	3287	1/1	0.82	0.95	51,51,51,51	0
56	MG	2A	3712	1/1	0.82	0.22	67,67,67,67	0
56	MG	2a	3165	1/1	0.82	0.23	78,78,78,78	0
56	MG	13	104	1/1	0.82	0.29	62,62,62,62	0
56	MG	2a	3183	1/1	0.82	0.15	58,58,58,58	0
56	MG	1a	1787	1/1	0.82	0.17	53,53,53,53	0
56	MG	1A	4025	1/1	0.82	0.28	74,74,74,74	0
56	MG	2A	3304	1/1	0.82	0.21	78,78,78,78	0
56	MG	2A	3780	1/1	0.82	0.12	70,70,70,70	0
56	MG	2A	3460	1/1	0.83	0.12	51,51,51,51	0
56	MG	1a	1696	1/1	0.83	0.17	61,61,61,61	0
56	MG	2A	3034	1/1	0.83	0.14	51,51,51,51	0
56	MG	2A	3512	1/1	0.83	0.21	69,69,69,69	0
56	MG	2A	3172	1/1	0.83	0.70	64,64,64,64	0
56	MG	1A	3426	1/1	0.83	0.14	51,51,51,51	0
56	MG	2A	3578	1/1	0.83	0.11	41,41,41,41	0
56	MG	2A	3592	1/1	0.83	0.27	61,61,61,61	0
56	MG	2a	3029	1/1	0.83	0.29	73,73,73,73	0
56	MG	2A	3593	1/1	0.83	0.22	73,73,73,73	0
56	MG	1a	1807	1/1	0.83	0.12	66,66,66,66	0
56	MG	1a	1603	1/1	0.83	0.48	54,54,54,54	0
56	MG	2A	3300	1/1	0.83	0.23	57,57,57,57	0
56	MG	1A	3345	1/1	0.83	0.42	46,46,46,46	0
56	MG	2A	3668	1/1	0.83	0.14	64,64,64,64	0
56	MG	2A	3195	1/1	0.83	0.60	76,76,76,76	0
56	MG	2A	3684	1/1	0.83	0.06	65,65,65,65	0
56	MG	1A	3454	1/1	0.83	0.31	48,48,48,48	0
56	MG	1a	1638	1/1	0.83	0.23	58,58,58,58	0
56	MG	2A	3224	1/1	0.83	0.35	53,53,53,53	0
56	MG	1a	1653	1/1	0.83	0.14	61,61,61,61	0
56	MG	1A	3391	1/1	0.83	0.13	53,53,53,53	0
56	MG	2A	3341	1/1	0.83	0.11	47,47,47,47	0
56	MG	1A	3320	1/1	0.83	0.13	51,51,51,51	0
56	MG	1A	3785	1/1	0.83	0.49	68,68,68,68	0
56	MG	2A	3239	1/1	0.83	0.21	66,66,66,66	0
56	MG	2A	3791	1/1	0.83	0.38	56,56,56,56	0
56	MG	1A	3464	1/1	0.83	1.01	57,57,57,57	0
56	MG	2B	207	1/1	0.83	0.11	55,55,55,55	0
56	MG	2A	3096	1/1	0.83	0.10	59,59,59,59	0
56	MG	2a	3192	1/1	0.83	0.13	70,70,70,70	0
56	MG	1a	1777	1/1	0.83	0.27	69,69,69,69	0
56	MG	1A	3167	1/1	0.83	0.37	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	2r	101	1/1	0.83	0.17	62,62,62,62	0
56	MG	2A	3143	1/1	0.83	0.98	59,59,59,59	0
56	MG	2A	3085	1/1	0.84	0.16	55,55,55,55	0
56	MG	2A	3090	1/1	0.84	0.16	38,38,38,38	0
56	MG	2A	3474	1/1	0.84	0.96	66,66,66,66	0
56	MG	1A	4017	1/1	0.84	0.12	54,54,54,54	0
56	MG	1A	3256	1/1	0.84	0.26	36,36,36,36	0
56	MG	2A	3112	1/1	0.84	1.00	63,63,63,63	0
56	MG	1A	3706	1/1	0.84	0.15	27,27,27,27	0
56	MG	2A	3570	1/1	0.84	0.14	51,51,51,51	0
56	MG	1B	221	1/1	0.84	0.22	66,66,66,66	0
56	MG	1A	3322	1/1	0.84	1.11	60,60,60,60	0
56	MG	2a	3044	1/1	0.84	0.45	54,54,54,54	0
56	MG	1A	3323	1/1	0.84	0.16	31,31,31,31	0
56	MG	1A	3349	1/1	0.84	0.33	56,56,56,56	0
56	MG	2A	3180	1/1	0.84	0.24	56,56,56,56	0
56	MG	1A	3471	1/1	0.84	0.12	50,50,50,50	0
56	MG	1A	3274	1/1	0.84	0.20	39,39,39,39	0
56	MG	2A	3308	1/1	0.84	0.30	74,74,74,74	0
56	MG	1A	3780	1/1	0.84	0.39	72,72,72,72	0
56	MG	2A	3313	1/1	0.84	0.33	52,52,52,52	0
56	MG	1A	3514	1/1	0.84	0.34	61,61,61,61	0
56	MG	2A	3698	1/1	0.84	0.40	54,54,54,54	0
56	MG	1A	3938	1/1	0.84	0.42	52,52,52,52	0
56	MG	1A	3381	1/1	0.84	0.38	60,60,60,60	0
56	MG	2A	3219	1/1	0.84	0.55	57,57,57,57	0
56	MG	1A	3382	1/1	0.84	0.30	55,55,55,55	0
56	MG	2A	3718	1/1	0.84	0.14	79,79,79,79	0
56	MG	1A	3120	1/1	0.84	0.21	40,40,40,40	0
56	MG	2a	3152	1/1	0.84	0.24	79,79,79,79	0
56	MG	1A	3576	1/1	0.84	0.14	34,34,34,34	0
56	MG	1A	3971	1/1	0.84	0.09	59,59,59,59	0
56	MG	1A	3029	1/1	0.84	0.18	51,51,51,51	0
56	MG	1A	3396	1/1	0.84	0.30	53,53,53,53	0
56	MG	2A	3392	1/1	0.84	0.32	56,56,56,56	0
56	MG	2A	3410	1/1	0.84	0.16	64,64,64,64	0
56	MG	1A	3870	1/1	0.84	0.17	62,62,62,62	0
56	MG	1A	3647	1/1	0.84	0.31	44,44,44,44	0
56	MG	2a	3216	1/1	0.84	0.34	67,67,67,67	0
56	MG	2A	3258	1/1	0.84	0.42	62,62,62,62	0
56	MG	2T	201	1/1	0.84	0.58	63,63,63,63	0
56	MG	2A	3242	1/1	0.85	0.26	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	1654	1/1	0.85	0.14	48,48,48,48	0
56	MG	2A	3251	1/1	0.85	0.68	63,63,63,63	0
56	MG	1A	3383	1/1	0.85	0.41	56,56,56,56	0
56	MG	2A	3451	1/1	0.85	0.14	51,51,51,51	0
56	MG	2A	3455	1/1	0.85	1.15	61,61,61,61	0
56	MG	2A	3260	1/1	0.85	0.53	62,62,62,62	0
56	MG	1a	1662	1/1	0.85	0.92	67,67,67,67	0
56	MG	1a	1663	1/1	0.85	0.15	70,70,70,70	0
56	MG	2A	3490	1/1	0.85	0.86	43,43,43,43	0
56	MG	1A	3384	1/1	0.85	0.48	48,48,48,48	0
56	MG	1A	3947	1/1	0.85	0.46	60,60,60,60	0
56	MG	1A	3027	1/1	0.85	0.15	69,69,69,69	0
56	MG	2A	3544	1/1	0.85	0.12	42,42,42,42	0
56	MG	1A	3661	1/1	0.85	0.13	69,69,69,69	0
56	MG	2a	3068	1/1	0.85	0.13	60,60,60,60	0
56	MG	1A	3968	1/1	0.85	0.09	80,80,80,80	0
56	MG	2A	3169	1/1	0.85	0.17	54,54,54,54	0
56	MG	1A	3918	1/1	0.85	0.14	47,47,47,47	0
56	MG	1X	104	1/1	0.85	0.27	44,44,44,44	0
56	MG	1x	112	1/1	0.85	0.16	68,68,68,68	0
56	MG	2A	3183	1/1	0.85	0.36	66,66,66,66	0
56	MG	2A	3623	1/1	0.85	0.13	55,55,55,55	0
56	MG	2A	3306	1/1	0.85	0.17	46,46,46,46	0
56	MG	2a	3117	1/1	0.85	0.25	53,53,53,53	0
56	MG	2a	3119	1/1	0.85	0.26	85,85,85,85	0
56	MG	1A	3213	1/1	0.85	0.27	56,56,56,56	0
56	MG	1a	1716	1/1	0.85	0.15	56,56,56,56	0
56	MG	1a	1718	1/1	0.85	0.28	46,46,46,46	0
56	MG	1A	3825	1/1	0.85	0.09	65,65,65,65	0
56	MG	2a	3130	1/1	0.85	0.30	100,100,100,100	0
56	MG	1A	3061	1/1	0.85	0.14	47,47,47,47	0
56	MG	2A	3200	1/1	0.85	0.51	47,47,47,47	0
56	MG	2a	3138	1/1	0.85	0.34	70,70,70,70	0
56	MG	2A	3699	1/1	0.85	0.41	69,69,69,69	0
56	MG	2A	3321	1/1	0.85	0.41	54,54,54,54	0
56	MG	1A	3718	1/1	0.85	0.22	39,39,39,39	0
56	MG	1A	3564	1/1	0.85	0.13	36,36,36,36	0
56	MG	2a	3158	1/1	0.85	0.25	71,71,71,71	0
56	MG	1a	1765	1/1	0.85	0.12	53,53,53,53	0
56	MG	1A	3182	1/1	0.85	0.12	53,53,53,53	0
56	MG	2a	3175	1/1	0.85	0.12	49,49,49,49	0
56	MG	1a	1623	1/1	0.85	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	4030	1/1	0.85	0.18	62,62,62,62	0
56	MG	1a	1643	1/1	0.85	0.42	71,71,71,71	0
56	MG	2a	3193	1/1	0.85	0.18	81,81,81,81	0
56	MG	1a	1644	1/1	0.85	0.17	66,66,66,66	0
56	MG	1A	3403	1/1	0.85	0.42	64,64,64,64	0
56	MG	2A	3396	1/1	0.85	0.16	45,45,45,45	0
56	MG	2A	3406	1/1	0.85	0.15	64,64,64,64	0
56	MG	2B	214	1/1	0.85	0.14	65,65,65,65	0
56	MG	1A	3685	1/1	0.86	0.50	59,59,59,59	0
56	MG	1O	201	1/1	0.86	0.30	43,43,43,43	0
56	MG	20	101	1/1	0.86	0.15	47,47,47,47	0
56	MG	1A	3104	1/1	0.86	0.25	33,33,33,33	0
56	MG	2A	3267	1/1	0.86	0.12	58,58,58,58	0
56	MG	2a	3005	1/1	0.86	0.29	60,60,60,60	0
56	MG	2A	3126	1/1	0.86	0.35	56,56,56,56	0
56	MG	2A	3271	1/1	0.86	0.10	59,59,59,59	0
56	MG	2A	3276	1/1	0.86	0.32	46,46,46,46	0
56	MG	1A	3713	1/1	0.86	0.14	36,36,36,36	0
56	MG	2A	3508	1/1	0.86	0.08	75,75,75,75	0
56	MG	1a	1681	1/1	0.86	2.19	62,62,62,62	0
56	MG	2A	3158	1/1	0.86	1.71	72,72,72,72	0
56	MG	2A	3526	1/1	0.86	0.39	75,75,75,75	0
56	MG	2a	3035	1/1	0.86	0.14	62,62,62,62	0
56	MG	1n	102	1/1	0.86	0.62	71,71,71,71	0
56	MG	1A	3425	1/1	0.86	0.23	73,73,73,73	0
56	MG	1A	3051	1/1	0.86	0.16	67,67,67,67	0
56	MG	1U	210	1/1	0.86	0.20	47,47,47,47	0
56	MG	2A	3586	1/1	0.86	0.13	66,66,66,66	0
56	MG	2A	3591	1/1	0.86	0.10	45,45,45,45	0
56	MG	2A	3173	1/1	0.86	0.12	58,58,58,58	0
56	MG	1A	3722	1/1	0.86	0.16	58,58,58,58	0
56	MG	2a	3108	1/1	0.86	0.12	73,73,73,73	0
56	MG	1Y	201	1/1	0.86	0.11	49,49,49,49	0
56	MG	2a	3111	1/1	0.86	0.23	89,89,89,89	0
56	MG	1A	3566	1/1	0.86	0.09	28,28,28,28	0
56	MG	2a	3115	1/1	0.86	0.15	64,64,64,64	0
56	MG	2A	3014	1/1	0.86	0.41	66,66,66,66	0
56	MG	1A	3132	1/1	0.86	0.17	25,25,25,25	0
56	MG	2A	3637	1/1	0.86	1.02	74,74,74,74	0
56	MG	1A	3212	1/1	0.86	0.42	50,50,50,50	0
56	MG	15	105	1/1	0.86	0.91	48,48,48,48	0
56	MG	2A	3317	1/1	0.86	0.30	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	3198	1/1	0.86	0.67	47,47,47,47	0
56	MG	1A	4010	1/1	0.86	0.07	49,49,49,49	0
56	MG	2A	3201	1/1	0.86	0.69	44,44,44,44	0
56	MG	1A	4013	1/1	0.86	0.06	43,43,43,43	0
56	MG	2A	3334	1/1	0.86	0.69	50,50,50,50	0
56	MG	1A	3358	1/1	0.86	0.24	33,33,33,33	0
56	MG	2A	3342	1/1	0.86	0.22	55,55,55,55	0
56	MG	2A	3053	1/1	0.86	0.62	57,57,57,57	0
56	MG	1A	3621	1/1	0.86	0.15	40,40,40,40	0
56	MG	1a	1767	1/1	0.86	0.17	54,54,54,54	0
56	MG	1A	3926	1/1	0.86	0.27	61,61,61,61	0
56	MG	2A	3736	1/1	0.86	0.23	60,60,60,60	0
56	MG	1A	3636	1/1	0.86	0.14	34,34,34,34	0
56	MG	1a	1773	1/1	0.86	0.11	63,63,63,63	0
56	MG	1A	3362	1/1	0.86	0.17	38,38,38,38	0
56	MG	1A	3276	1/1	0.86	0.56	51,51,51,51	0
56	MG	2A	3408	1/1	0.86	0.16	44,44,44,44	0
56	MG	1A	3287	1/1	0.86	0.29	36,36,36,36	0
56	MG	2E	302	1/1	0.86	0.99	52,52,52,52	0
56	MG	1A	3682	1/1	0.86	0.19	64,64,64,64	0
56	MG	1E	301	1/1	0.86	0.59	45,45,45,45	0
56	MG	2A	3049	1/1	0.87	0.14	47,47,47,47	0
56	MG	1A	3340	1/1	0.87	0.37	61,61,61,61	0
56	MG	1A	3941	1/1	0.87	0.32	55,55,55,55	0
56	MG	1A	3319	1/1	0.87	0.17	30,30,30,30	0
56	MG	1E	307	1/1	0.87	0.20	38,38,38,38	0
56	MG	1A	3662	1/1	0.87	0.25	68,68,68,68	0
56	MG	1A	3893	1/1	0.87	0.15	51,51,51,51	0
56	MG	2A	3071	1/1	0.87	0.18	64,64,64,64	0
56	MG	1a	1666	1/1	0.87	0.41	66,66,66,66	0
56	MG	1A	3895	1/1	0.87	0.10	72,72,72,72	0
56	MG	1A	3565	1/1	0.87	0.13	41,41,41,41	0
56	MG	1A	3289	1/1	0.87	0.17	36,36,36,36	0
56	MG	2A	3688	1/1	0.87	0.25	63,63,63,63	0
56	MG	2a	3096	1/1	0.87	0.30	64,64,64,64	0
56	MG	1A	3974	1/1	0.87	0.08	75,75,75,75	0
56	MG	2A	3244	1/1	0.87	0.18	64,64,64,64	0
56	MG	1A	3978	1/1	0.87	0.24	77,77,77,77	0
56	MG	2A	3099	1/1	0.87	0.10	64,64,64,64	0
56	MG	2A	3255	1/1	0.87	1.08	50,50,50,50	0
56	MG	1l	203	1/1	0.87	0.17	61,61,61,61	0
56	MG	1m	201	1/1	0.87	0.31	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3124	1/1	0.87	0.12	50,50,50,50	0
56	MG	2A	3719	1/1	0.87	0.43	74,74,74,74	0
56	MG	1A	3922	1/1	0.87	0.18	83,83,83,83	0
56	MG	1A	3066	1/1	0.87	0.29	54,54,54,54	0
56	MG	2A	3444	1/1	0.87	0.15	54,54,54,54	0
56	MG	2A	3142	1/1	0.87	0.71	39,39,39,39	0
56	MG	1A	3578	1/1	0.87	0.14	37,37,37,37	0
56	MG	1x	108	1/1	0.87	0.13	64,64,64,64	0
56	MG	2a	3137	1/1	0.87	0.12	66,66,66,66	0
56	MG	1A	3826	1/1	0.87	0.10	45,45,45,45	0
56	MG	1A	3184	1/1	0.87	0.19	40,40,40,40	0
56	MG	1A	3063	1/1	0.87	0.60	60,60,60,60	0
56	MG	2E	301	1/1	0.87	0.66	62,62,62,62	0
56	MG	2A	3483	1/1	0.87	0.23	56,56,56,56	0
56	MG	1A	3933	1/1	0.87	0.17	38,38,38,38	0
56	MG	1A	3133	1/1	0.87	0.18	46,46,46,46	0
56	MG	2A	3177	1/1	0.87	0.48	46,46,46,46	0
56	MG	1a	1608	1/1	0.87	0.14	60,60,60,60	0
56	MG	2Y	201	1/1	0.87	0.21	49,49,49,49	0
56	MG	2A	3299	1/1	0.87	0.46	48,48,48,48	0
56	MG	1A	4028	1/1	0.87	0.21	52,52,52,52	0
56	MG	1A	3312	1/1	0.87	0.27	64,64,64,64	0
56	MG	1A	4035	1/1	0.87	0.12	46,46,46,46	0
56	MG	1a	1639	1/1	0.87	0.21	47,47,47,47	0
56	MG	1A	3118	1/1	0.87	0.57	48,48,48,48	0
56	MG	2A	3046	1/1	0.87	0.47	73,73,73,73	0
56	MG	2a	3019	1/1	0.87	0.11	59,59,59,59	0
56	MG	1A	3479	1/1	0.88	0.19	37,37,37,37	0
56	MG	1A	3607	1/1	0.88	0.17	42,42,42,42	0
56	MG	2A	3360	1/1	0.88	0.29	71,71,71,71	0
56	MG	2A	3361	1/1	0.88	0.13	53,53,53,53	0
56	MG	2A	3050	1/1	0.88	0.20	50,50,50,50	0
56	MG	2B	204	1/1	0.88	0.29	61,61,61,61	0
56	MG	2B	206	1/1	0.88	0.23	57,57,57,57	0
56	MG	1A	4008	1/1	0.88	0.08	40,40,40,40	0
56	MG	1A	3909	1/1	0.88	0.21	55,55,55,55	0
56	MG	1A	3086	1/1	0.88	0.21	51,51,51,51	0
56	MG	1A	3624	1/1	0.88	0.20	30,30,30,30	0
56	MG	2A	3407	1/1	0.88	0.09	49,49,49,49	0
56	MG	1A	3351	1/1	0.88	0.91	64,64,64,64	0
56	MG	2A	3241	1/1	0.88	0.16	40,40,40,40	0
56	MG	2P	202	1/1	0.88	0.36	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2R	201	1/1	0.88	0.83	48,48,48,48	0
56	MG	1A	3355	1/1	0.88	0.15	41,41,41,41	0
56	MG	2A	3440	1/1	0.88	0.12	49,49,49,49	0
56	MG	1a	1618	1/1	0.88	0.08	53,53,53,53	0
56	MG	2A	3073	1/1	0.88	1.14	55,55,55,55	0
56	MG	2A	3250	1/1	0.88	0.14	61,61,61,61	0
56	MG	1a	1620	1/1	0.88	0.30	65,65,65,65	0
56	MG	2A	3453	1/1	0.88	0.17	47,47,47,47	0
56	MG	2A	3252	1/1	0.88	0.43	54,54,54,54	0
56	MG	1a	1779	1/1	0.88	0.25	59,59,59,59	0
56	MG	2a	3014	1/1	0.88	0.19	66,66,66,66	0
56	MG	2a	3018	1/1	0.88	0.34	52,52,52,52	0
56	MG	2A	3467	1/1	0.88	0.23	61,61,61,61	0
56	MG	1A	4022	1/1	0.88	0.88	42,42,42,42	0
56	MG	2A	3473	1/1	0.88	0.10	58,58,58,58	0
56	MG	1A	3311	1/1	0.88	0.23	46,46,46,46	0
56	MG	2A	3261	1/1	0.88	0.26	46,46,46,46	0
56	MG	1a	1794	1/1	0.88	0.21	60,60,60,60	0
56	MG	1A	3820	1/1	0.88	0.58	45,45,45,45	0
56	MG	2A	3266	1/1	0.88	0.18	38,38,38,38	0
56	MG	2a	3048	1/1	0.88	0.57	74,74,74,74	0
56	MG	2a	3061	1/1	0.88	0.30	63,63,63,63	0
56	MG	1A	3540	1/1	0.88	0.34	42,42,42,42	0
56	MG	2A	3109	1/1	0.88	0.52	75,75,75,75	0
56	MG	1A	3360	1/1	0.88	0.76	53,53,53,53	0
56	MG	2A	3534	1/1	0.88	0.12	38,38,38,38	0
56	MG	1A	3257	1/1	0.88	0.20	70,70,70,70	0
56	MG	2A	3555	1/1	0.88	0.20	71,71,71,71	0
56	MG	1A	3828	1/1	0.88	0.16	64,64,64,64	0
56	MG	2a	3102	1/1	0.88	0.18	62,62,62,62	0
56	MG	2A	3278	1/1	0.88	0.12	56,56,56,56	0
56	MG	1A	3829	1/1	0.88	0.31	34,34,34,34	0
56	MG	2A	3280	1/1	0.88	0.20	43,43,43,43	0
56	MG	1B	226	1/1	0.88	0.15	51,51,51,51	0
56	MG	2a	3113	1/1	0.88	0.11	43,43,43,43	0
56	MG	1l	202	1/1	0.88	0.17	52,52,52,52	0
56	MG	1B	227	1/1	0.88	0.26	77,77,77,77	0
56	MG	2a	3116	1/1	0.88	0.11	74,74,74,74	0
56	MG	2A	3291	1/1	0.88	0.18	44,44,44,44	0
56	MG	2a	3118	1/1	0.88	0.29	48,48,48,48	0
56	MG	2A	3606	1/1	0.88	0.06	48,48,48,48	0
56	MG	1B	229	1/1	0.88	0.55	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3616	1/1	0.88	0.42	69,69,69,69	0
56	MG	1A	3830	1/1	0.88	0.14	27,27,27,27	0
56	MG	1A	3405	1/1	0.88	0.41	40,40,40,40	0
56	MG	1F	304	1/1	0.88	0.36	47,47,47,47	0
56	MG	2A	3640	1/1	0.88	0.06	75,75,75,75	0
56	MG	1A	3842	1/1	0.88	0.52	40,40,40,40	0
56	MG	1a	1684	1/1	0.88	0.17	40,40,40,40	0
56	MG	2A	3673	1/1	0.88	0.32	59,59,59,59	0
56	MG	2a	3141	1/1	0.88	0.06	61,61,61,61	0
56	MG	2A	3674	1/1	0.88	0.10	63,63,63,63	0
56	MG	1A	3342	1/1	0.88	0.23	45,45,45,45	0
56	MG	1A	3097	1/1	0.88	0.50	59,59,59,59	0
56	MG	1a	1707	1/1	0.88	0.13	61,61,61,61	0
56	MG	2a	3156	1/1	0.88	0.27	76,76,76,76	0
56	MG	2A	3002	1/1	0.88	0.14	41,41,41,41	0
56	MG	1A	3308	1/1	0.88	0.18	46,46,46,46	0
56	MG	1A	3716	1/1	0.88	0.22	28,28,28,28	0
56	MG	2A	3026	1/1	0.88	0.12	39,39,39,39	0
56	MG	1A	3970	1/1	0.88	0.06	79,79,79,79	0
56	MG	2A	3713	1/1	0.88	0.31	58,58,58,58	0
56	MG	1A	3587	1/1	0.88	0.11	49,49,49,49	0
56	MG	2A	3199	1/1	0.88	0.13	52,52,52,52	0
56	MG	2a	3200	1/1	0.88	0.16	73,73,73,73	0
56	MG	2a	3206	1/1	0.88	0.09	63,63,63,63	0
56	MG	1a	1717	1/1	0.88	0.15	62,62,62,62	0
56	MG	1A	3333	1/1	0.88	1.32	45,45,45,45	0
56	MG	2A	3720	1/1	0.88	0.24	48,48,48,48	0
56	MG	1A	3596	1/1	0.88	0.21	38,38,38,38	0
56	MG	2v	101	1/1	0.88	0.48	77,77,77,77	0
56	MG	2A	3211	1/1	0.88	0.31	44,44,44,44	0
56	MG	1A	3988	1/1	0.89	0.11	50,50,50,50	0
56	MG	2A	3415	1/1	0.89	0.68	43,43,43,43	0
56	MG	1A	3993	1/1	0.89	0.09	85,85,85,85	0
56	MG	1A	3532	1/1	0.89	0.64	42,42,42,42	0
56	MG	1A	3886	1/1	0.89	0.13	45,45,45,45	0
56	MG	1A	3270	1/1	0.89	0.37	49,49,49,49	0
56	MG	1A	3364	1/1	0.89	0.32	44,44,44,44	0
56	MG	1A	3545	1/1	0.89	0.28	58,58,58,58	0
56	MG	2A	3256	1/1	0.89	1.50	57,57,57,57	0
56	MG	2A	3454	1/1	0.89	0.13	53,53,53,53	0
56	MG	1A	3272	1/1	0.89	0.33	42,42,42,42	0
56	MG	2R	202	1/1	0.89	1.74	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	3457	1/1	0.89	0.17	48,48,48,48	0
56	MG	2A	3458	1/1	0.89	0.20	38,38,38,38	0
56	MG	1a	1774	1/1	0.89	0.12	67,67,67,67	0
56	MG	2A	3464	1/1	0.89	0.23	75,75,75,75	0
56	MG	2a	3002	1/1	0.89	0.32	74,74,74,74	0
56	MG	1A	3557	1/1	0.89	0.17	34,34,34,34	0
56	MG	1A	4020	1/1	0.89	0.18	42,42,42,42	0
56	MG	1a	1786	1/1	0.89	0.18	75,75,75,75	0
56	MG	1a	1624	1/1	0.89	0.70	68,68,68,68	0
56	MG	2a	3009	1/1	0.89	0.31	74,74,74,74	0
56	MG	2A	3475	1/1	0.89	0.16	50,50,50,50	0
56	MG	1A	3434	1/1	0.89	0.21	39,39,39,39	0
56	MG	2a	3017	1/1	0.89	0.52	53,53,53,53	0
56	MG	2A	3484	1/1	0.89	0.58	63,63,63,63	0
56	MG	1A	3921	1/1	0.89	0.10	63,63,63,63	0
56	MG	1A	3735	1/1	0.89	0.12	35,35,35,35	0
56	MG	2A	3494	1/1	0.89	0.06	69,69,69,69	0
56	MG	1A	3380	1/1	0.89	0.63	42,42,42,42	0
56	MG	2A	3115	1/1	0.89	0.16	57,57,57,57	0
56	MG	2a	3025	1/1	0.89	0.71	63,63,63,63	0
56	MG	2A	3521	1/1	0.89	0.07	52,52,52,52	0
56	MG	1A	3081	1/1	0.89	0.35	41,41,41,41	0
56	MG	1a	1814	1/1	0.89	0.09	63,63,63,63	0
56	MG	2A	3527	1/1	0.89	0.34	55,55,55,55	0
56	MG	1A	3017	1/1	0.89	0.23	44,44,44,44	0
56	MG	2A	3542	1/1	0.89	0.38	69,69,69,69	0
56	MG	2a	3071	1/1	0.89	0.13	59,59,59,59	0
56	MG	1A	3191	1/1	0.89	0.18	46,46,46,46	0
56	MG	1A	3584	1/1	0.89	0.18	40,40,40,40	0
56	MG	2a	3083	1/1	0.89	0.10	57,57,57,57	0
56	MG	2A	3557	1/1	0.89	0.33	61,61,61,61	0
56	MG	1A	3240	1/1	0.89	0.18	41,41,41,41	0
56	MG	2A	3566	1/1	0.89	0.14	66,66,66,66	0
56	MG	1A	3790	1/1	0.89	0.13	50,50,50,50	0
56	MG	2A	3573	1/1	0.89	0.52	66,66,66,66	0
56	MG	2A	3168	1/1	0.89	0.19	44,44,44,44	0
56	MG	2A	3585	1/1	0.89	0.12	60,60,60,60	0
56	MG	1A	3252	1/1	0.89	0.41	59,59,59,59	0
56	MG	1A	3025	1/1	0.89	0.57	55,55,55,55	0
56	MG	1n	101	1/1	0.89	0.13	51,51,51,51	0
56	MG	1a	1671	1/1	0.89	0.45	47,47,47,47	0
56	MG	1A	3395	1/1	0.89	0.61	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	3178	1/1	0.89	0.21	52,52,52,52	0
56	MG	2A	3179	1/1	0.89	0.16	63,63,63,63	0
56	MG	1a	1680	1/1	0.89	0.20	60,60,60,60	0
56	MG	1x	107	1/1	0.89	0.33	67,67,67,67	0
56	MG	1E	308	1/1	0.89	0.12	26,26,26,26	0
56	MG	1A	3293	1/1	0.89	0.17	35,35,35,35	0
56	MG	1a	1686	1/1	0.89	0.13	50,50,50,50	0
56	MG	2A	3646	1/1	0.89	0.14	71,71,71,71	0
56	MG	1A	3397	1/1	0.89	0.91	58,58,58,58	0
56	MG	1A	3353	1/1	0.89	0.22	52,52,52,52	0
56	MG	2A	3327	1/1	0.89	0.13	70,70,70,70	0
56	MG	1A	3302	1/1	0.89	0.48	52,52,52,52	0
56	MG	2A	3009	1/1	0.89	0.34	57,57,57,57	0
56	MG	2A	3338	1/1	0.89	1.07	55,55,55,55	0
56	MG	2A	3010	1/1	0.89	0.16	56,56,56,56	0
56	MG	1Q	202	1/1	0.89	0.30	45,45,45,45	0
56	MG	2A	3347	1/1	0.89	0.16	45,45,45,45	0
56	MG	1A	3638	1/1	0.89	0.23	32,32,32,32	0
56	MG	1a	1713	1/1	0.89	0.44	41,41,41,41	0
56	MG	2A	3355	1/1	0.89	0.16	51,51,51,51	0
56	MG	1A	3203	1/1	0.89	0.31	47,47,47,47	0
56	MG	1A	3497	1/1	0.89	0.13	43,43,43,43	0
56	MG	1A	3504	1/1	0.89	0.34	55,55,55,55	0
56	MG	2a	3181	1/1	0.89	0.19	64,64,64,64	0
56	MG	2A	3362	1/1	0.89	0.16	54,54,54,54	0
56	MG	2A	3363	1/1	0.89	0.12	63,63,63,63	0
56	MG	1A	3509	1/1	0.89	0.26	65,65,65,65	0
56	MG	2A	3369	1/1	0.89	0.13	63,63,63,63	0
56	MG	2a	3196	1/1	0.89	0.37	64,64,64,64	0
56	MG	1A	3305	1/1	0.89	0.30	49,49,49,49	0
56	MG	2A	3229	1/1	0.89	0.15	39,39,39,39	0
56	MG	2A	3754	1/1	0.89	0.26	63,63,63,63	0
56	MG	2A	3776	1/1	0.89	0.15	62,62,62,62	0
56	MG	2a	3215	1/1	0.89	0.17	75,75,75,75	0
56	MG	1a	1727	1/1	0.89	0.26	52,52,52,52	0
56	MG	1a	1728	1/1	0.89	0.43	62,62,62,62	0
56	MG	1a	1731	1/1	0.89	0.17	62,62,62,62	0
56	MG	1A	3410	1/1	0.89	0.22	29,29,29,29	0
56	MG	2A	3388	1/1	0.90	1.11	52,52,52,52	0
56	MG	2A	3194	1/1	0.90	0.46	63,63,63,63	0
56	MG	2A	3787	1/1	0.90	0.07	69,69,69,69	0
56	MG	1A	3423	1/1	0.90	0.95	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	3863	1/1	0.90	0.18	57,57,57,57	0
56	MG	1a	1642	1/1	0.90	0.35	42,42,42,42	0
56	MG	1A	3997	1/1	0.90	0.42	63,63,63,63	0
56	MG	1A	3673	1/1	0.90	0.19	50,50,50,50	0
56	MG	2A	3412	1/1	0.90	0.21	57,57,57,57	0
56	MG	1A	3867	1/1	0.90	0.20	78,78,78,78	0
56	MG	2A	3430	1/1	0.90	0.12	42,42,42,42	0
56	MG	1x	104	1/1	0.90	0.28	64,64,64,64	0
56	MG	2E	305	1/1	0.90	0.30	42,42,42,42	0
56	MG	2A	3436	1/1	0.90	0.20	51,51,51,51	0
56	MG	1A	4012	1/1	0.90	0.19	56,56,56,56	0
56	MG	2A	3220	1/1	0.90	0.38	58,58,58,58	0
56	MG	1A	3273	1/1	0.90	0.11	43,43,43,43	0
56	MG	1A	3525	1/1	0.90	0.26	42,42,42,42	0
56	MG	2A	3447	1/1	0.90	0.32	44,44,44,44	0
56	MG	1A	3696	1/1	0.90	0.20	48,48,48,48	0
56	MG	1A	3875	1/1	0.90	0.19	57,57,57,57	0
56	MG	1x	114	1/1	0.90	0.16	71,71,71,71	0
56	MG	2A	3232	1/1	0.90	0.47	55,55,55,55	0
56	MG	1A	3880	1/1	0.90	0.17	56,56,56,56	0
56	MG	1A	3232	1/1	0.90	0.63	45,45,45,45	0
56	MG	1A	3149	1/1	0.90	1.43	40,40,40,40	0
56	MG	1A	4027	1/1	0.90	0.21	56,56,56,56	0
56	MG	2A	3013	1/1	0.90	0.32	44,44,44,44	0
56	MG	1A	3285	1/1	0.90	0.22	42,42,42,42	0
56	MG	2a	3013	1/1	0.90	0.17	68,68,68,68	0
56	MG	1A	3286	1/1	0.90	0.22	41,41,41,41	0
56	MG	1a	1683	1/1	0.90	0.13	61,61,61,61	0
56	MG	1A	3238	1/1	0.90	0.15	63,63,63,63	0
56	MG	2A	3476	1/1	0.90	0.37	55,55,55,55	0
56	MG	1A	4039	1/1	0.90	0.51	76,76,76,76	0
56	MG	1A	3721	1/1	0.90	0.09	31,31,31,31	0
56	MG	2A	3037	1/1	0.90	0.13	50,50,50,50	0
56	MG	1a	1692	1/1	0.90	0.57	70,70,70,70	0
56	MG	1a	1695	1/1	0.90	0.22	69,69,69,69	0
56	MG	2a	3028	1/1	0.90	0.29	61,61,61,61	0
56	MG	1B	210	1/1	0.90	0.24	49,49,49,49	0
56	MG	2A	3047	1/1	0.90	0.23	53,53,53,53	0
56	MG	1A	3389	1/1	0.90	0.40	52,52,52,52	0
56	MG	1A	3724	1/1	0.90	0.12	33,33,33,33	0
56	MG	2a	3059	1/1	0.90	0.15	40,40,40,40	0
56	MG	1A	3561	1/1	0.90	0.23	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	3314	1/1	0.90	0.24	43,43,43,43	0
56	MG	1B	228	1/1	0.90	0.13	51,51,51,51	0
56	MG	2A	3537	1/1	0.90	0.08	52,52,52,52	0
56	MG	1A	3316	1/1	0.90	0.19	42,42,42,42	0
56	MG	1A	3453	1/1	0.90	0.35	47,47,47,47	0
56	MG	2a	3086	1/1	0.90	0.11	63,63,63,63	0
56	MG	2a	3089	1/1	0.90	0.13	53,53,53,53	0
56	MG	1A	3749	1/1	0.90	0.12	41,41,41,41	0
56	MG	1A	3318	1/1	0.90	0.14	58,58,58,58	0
56	MG	1F	303	1/1	0.90	0.95	43,43,43,43	0
56	MG	1A	3756	1/1	0.90	0.30	39,39,39,39	0
56	MG	2a	3100	1/1	0.90	0.11	76,76,76,76	0
56	MG	1a	1730	1/1	0.90	0.11	80,80,80,80	0
56	MG	1F	308	1/1	0.90	0.14	32,32,32,32	0
56	MG	2a	3106	1/1	0.90	0.12	63,63,63,63	0
56	MG	1A	3935	1/1	0.90	0.28	46,46,46,46	0
56	MG	1A	3116	1/1	0.90	0.30	43,43,43,43	0
56	MG	1a	1741	1/1	0.90	0.24	54,54,54,54	0
56	MG	2A	3297	1/1	0.90	0.60	54,54,54,54	0
56	MG	1a	1761	1/1	0.90	0.07	47,47,47,47	0
56	MG	2A	3102	1/1	0.90	0.21	50,50,50,50	0
56	MG	1a	1762	1/1	0.90	0.14	44,44,44,44	0
56	MG	1A	3175	1/1	0.90	0.24	55,55,55,55	0
56	MG	1A	3399	1/1	0.90	0.16	42,42,42,42	0
56	MG	1A	3197	1/1	0.90	0.13	47,47,47,47	0
56	MG	2A	3121	1/1	0.90	0.29	49,49,49,49	0
56	MG	1A	3813	1/1	0.90	0.12	48,48,48,48	0
56	MG	2A	3314	1/1	0.90	0.32	52,52,52,52	0
56	MG	1A	3468	1/1	0.90	0.51	37,37,37,37	0
56	MG	1A	3470	1/1	0.90	1.34	32,32,32,32	0
56	MG	2A	3647	1/1	0.90	0.09	72,72,72,72	0
56	MG	1A	3215	1/1	0.90	0.31	53,53,53,53	0
56	MG	1A	3956	1/1	0.90	0.18	36,36,36,36	0
56	MG	2A	3671	1/1	0.90	0.10	45,45,45,45	0
56	MG	2A	3323	1/1	0.90	0.57	42,42,42,42	0
56	MG	2A	3156	1/1	0.90	0.13	70,70,70,70	0
56	MG	1A	3961	1/1	0.90	0.18	40,40,40,40	0
56	MG	2a	3147	1/1	0.90	0.32	70,70,70,70	0
56	MG	1A	3221	1/1	0.90	0.42	35,35,35,35	0
56	MG	1A	3407	1/1	0.90	0.22	56,56,56,56	0
56	MG	2A	3691	1/1	0.90	0.66	68,68,68,68	0
56	MG	2A	3692	1/1	0.90	0.27	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3229	1/1	0.90	0.14	46,46,46,46	0
56	MG	1a	1602	1/1	0.90	0.18	74,74,74,74	0
56	MG	1A	3499	1/1	0.90	0.30	51,51,51,51	0
56	MG	2a	3178	1/1	0.90	0.22	69,69,69,69	0
56	MG	1A	3973	1/1	0.90	0.06	78,78,78,78	0
56	MG	1a	1607	1/1	0.90	0.52	64,64,64,64	0
56	MG	1A	3409	1/1	0.90	0.29	46,46,46,46	0
56	MG	2a	3191	1/1	0.90	0.58	67,67,67,67	0
56	MG	1A	3506	1/1	0.90	0.16	38,38,38,38	0
56	MG	1a	1613	1/1	0.90	0.20	71,71,71,71	0
56	MG	1a	1821	1/1	0.90	0.11	49,49,49,49	0
56	MG	1A	3331	1/1	0.90	1.16	45,45,45,45	0
56	MG	2A	3185	1/1	0.90	0.21	46,46,46,46	0
56	MG	2a	3208	1/1	0.90	0.07	66,66,66,66	0
56	MG	1A	3984	1/1	0.90	0.12	65,65,65,65	0
56	MG	2a	3213	1/1	0.90	0.31	70,70,70,70	0
56	MG	2A	3729	1/1	0.90	0.23	66,66,66,66	0
56	MG	1A	3987	1/1	0.90	0.41	49,49,49,49	0
56	MG	2A	3734	1/1	0.90	0.10	45,45,45,45	0
56	MG	2a	3217	1/1	0.90	0.09	76,76,76,76	0
56	MG	2d	301	1/1	0.90	0.17	59,59,59,59	0
56	MG	2q	201	1/1	0.90	0.19	60,60,60,60	0
56	MG	1A	3854	1/1	0.90	0.41	52,52,52,52	0
56	MG	2A	3385	1/1	0.90	0.16	51,51,51,51	0
56	MG	2A	3193	1/1	0.90	0.28	63,63,63,63	0
59	K	2A	3421	1/1	0.90	0.95	91,91,91,91	0
56	MG	1A	3917	1/1	0.91	0.08	72,72,72,72	0
56	MG	1A	3246	1/1	0.91	0.14	31,31,31,31	0
56	MG	2A	3711	1/1	0.91	0.06	67,67,67,67	0
56	MG	1a	1714	1/1	0.91	0.21	54,54,54,54	0
56	MG	1A	3156	1/1	0.91	0.08	61,61,61,61	0
56	MG	1A	3254	1/1	0.91	0.38	55,55,55,55	0
56	MG	2A	3086	1/1	0.91	0.22	49,49,49,49	0
56	MG	1D	310	1/1	0.91	0.55	36,36,36,36	0
56	MG	1A	3743	1/1	0.91	0.15	27,27,27,27	0
56	MG	2A	3097	1/1	0.91	0.18	51,51,51,51	0
56	MG	2A	3322	1/1	0.91	0.13	51,51,51,51	0
56	MG	2A	3725	1/1	0.91	0.46	60,60,60,60	0
56	MG	1a	1719	1/1	0.91	0.27	45,45,45,45	0
56	MG	2A	3732	1/1	0.91	0.40	74,74,74,74	0
56	MG	2A	3101	1/1	0.91	0.12	56,56,56,56	0
56	MG	1E	303	1/1	0.91	0.91	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	3105	1/1	0.91	0.39	57,57,57,57	0
56	MG	2A	3738	1/1	0.91	0.10	47,47,47,47	0
56	MG	1A	3206	1/1	0.91	0.21	44,44,44,44	0
56	MG	2A	3766	1/1	0.91	0.10	65,65,65,65	0
56	MG	2A	3773	1/1	0.91	0.34	67,67,67,67	0
56	MG	1A	3024	1/1	0.91	0.11	44,44,44,44	0
56	MG	1A	3579	1/1	0.91	0.12	45,45,45,45	0
56	MG	2A	3114	1/1	0.91	0.17	53,53,53,53	0
56	MG	1A	3005	1/1	0.91	0.40	42,42,42,42	0
56	MG	2A	3789	1/1	0.91	0.26	52,52,52,52	0
56	MG	2A	3348	1/1	0.91	0.09	57,57,57,57	0
56	MG	1F	305	1/1	0.91	0.12	51,51,51,51	0
56	MG	2A	3123	1/1	0.91	0.15	51,51,51,51	0
56	MG	2A	3353	1/1	0.91	0.73	44,44,44,44	0
56	MG	1a	1735	1/1	0.91	0.10	46,46,46,46	0
56	MG	1A	3762	1/1	0.91	0.17	51,51,51,51	0
56	MG	1G	201	1/1	0.91	0.08	50,50,50,50	0
56	MG	1a	1747	1/1	0.91	0.23	59,59,59,59	0
56	MG	1a	1751	1/1	0.91	0.12	73,73,73,73	0
56	MG	1A	3775	1/1	0.91	0.14	51,51,51,51	0
56	MG	2A	3157	1/1	0.91	0.22	42,42,42,42	0
56	MG	1A	3400	1/1	0.91	0.26	54,54,54,54	0
56	MG	2A	3380	1/1	0.91	0.12	44,44,44,44	0
56	MG	2Q	202	1/1	0.91	0.13	34,34,34,34	0
56	MG	1A	3126	1/1	0.91	0.12	44,44,44,44	0
56	MG	2A	3165	1/1	0.91	0.19	42,42,42,42	0
56	MG	2A	3387	1/1	0.91	0.25	49,49,49,49	0
56	MG	2W	202	1/1	0.91	0.12	47,47,47,47	0
56	MG	1A	3216	1/1	0.91	0.34	55,55,55,55	0
56	MG	1A	3047	1/1	0.91	0.19	44,44,44,44	0
56	MG	1A	3801	1/1	0.91	0.39	83,83,83,83	0
56	MG	23	101	1/1	0.91	0.74	37,37,37,37	0
56	MG	25	101	1/1	0.91	0.14	53,53,53,53	0
56	MG	25	104	1/1	0.91	0.53	61,61,61,61	0
56	MG	1T	204	1/1	0.91	0.15	35,35,35,35	0
56	MG	1T	205	1/1	0.91	0.31	55,55,55,55	0
56	MG	1A	3806	1/1	0.91	1.77	45,45,45,45	0
56	MG	1U	209	1/1	0.91	0.34	47,47,47,47	0
56	MG	1A	3602	1/1	0.91	0.48	37,37,37,37	0
56	MG	1A	3189	1/1	0.91	0.09	31,31,31,31	0
56	MG	2A	3417	1/1	0.91	0.74	42,42,42,42	0
56	MG	2A	3420	1/1	0.91	0.12	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	3181	1/1	0.91	0.25	49,49,49,49	0
56	MG	1A	3495	1/1	0.91	0.73	64,64,64,64	0
56	MG	10	101	1/1	0.91	0.26	42,42,42,42	0
56	MG	1A	3957	1/1	0.91	0.13	31,31,31,31	0
56	MG	1A	3496	1/1	0.91	0.22	60,60,60,60	0
56	MG	1a	1795	1/1	0.91	0.51	86,86,86,86	0
56	MG	13	102	1/1	0.91	0.34	41,41,41,41	0
56	MG	1a	1798	1/1	0.91	0.09	72,72,72,72	0
56	MG	1A	3626	1/1	0.91	0.12	39,39,39,39	0
56	MG	2a	3027	1/1	0.91	0.10	52,52,52,52	0
56	MG	1A	3965	1/1	0.91	0.07	76,76,76,76	0
56	MG	1a	1810	1/1	0.91	0.12	75,75,75,75	0
56	MG	16	102	1/1	0.91	0.73	50,50,50,50	0
56	MG	17	105	1/1	0.91	0.59	42,42,42,42	0
56	MG	17	107	1/1	0.91	0.17	29,29,29,29	0
56	MG	2a	3050	1/1	0.91	0.19	68,68,68,68	0
56	MG	2A	3203	1/1	0.91	0.33	45,45,45,45	0
56	MG	2A	3208	1/1	0.91	0.25	48,48,48,48	0
56	MG	1a	1601	1/1	0.91	0.13	65,65,65,65	0
56	MG	1A	3022	1/1	0.91	0.35	35,35,35,35	0
56	MG	2A	3218	1/1	0.91	1.06	64,64,64,64	0
56	MG	1A	3359	1/1	0.91	0.16	42,42,42,42	0
56	MG	2a	3080	1/1	0.91	0.51	54,54,54,54	0
56	MG	1A	3644	1/1	0.91	0.29	55,55,55,55	0
56	MG	1A	3233	1/1	0.91	0.17	57,57,57,57	0
56	MG	1A	3652	1/1	0.91	0.55	52,52,52,52	0
56	MG	1A	3419	1/1	0.91	0.85	43,43,43,43	0
56	MG	2A	3486	1/1	0.91	0.13	49,49,49,49	0
56	MG	1A	3234	1/1	0.91	0.16	56,56,56,56	0
56	MG	1A	3856	1/1	0.91	0.59	33,33,33,33	0
56	MG	1A	3985	1/1	0.91	0.15	45,45,45,45	0
56	MG	2A	3499	1/1	0.91	0.16	64,64,64,64	0
56	MG	2A	3233	1/1	0.91	0.11	59,59,59,59	0
56	MG	1A	3143	1/1	0.91	0.98	47,47,47,47	0
56	MG	1A	3671	1/1	0.91	0.15	51,51,51,51	0
56	MG	1a	1633	1/1	0.91	0.11	49,49,49,49	0
56	MG	1a	1636	1/1	0.91	0.17	49,49,49,49	0
56	MG	1A	3989	1/1	0.91	0.13	52,52,52,52	0
56	MG	1A	3864	1/1	0.91	0.21	56,56,56,56	0
56	MG	1A	3865	1/1	0.91	0.09	77,77,77,77	0
56	MG	2A	3538	1/1	0.91	0.07	57,57,57,57	0
56	MG	1A	3076	1/1	0.91	0.17	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	4007	1/1	0.91	0.23	55,55,55,55	0
56	MG	2A	3007	1/1	0.91	0.21	49,49,49,49	0
56	MG	2A	3253	1/1	0.91	0.20	49,49,49,49	0
56	MG	2A	3559	1/1	0.91	0.10	51,51,51,51	0
56	MG	1a	1645	1/1	0.91	0.25	65,65,65,65	0
56	MG	2a	3126	1/1	0.91	0.34	84,84,84,84	0
56	MG	1A	3519	1/1	0.91	0.39	44,44,44,44	0
56	MG	1A	3379	1/1	0.91	0.91	52,52,52,52	0
56	MG	2a	3133	1/1	0.91	0.23	78,78,78,78	0
56	MG	1A	3530	1/1	0.91	0.46	37,37,37,37	0
56	MG	1A	3872	1/1	0.91	0.10	50,50,50,50	0
56	MG	2A	3024	1/1	0.91	0.95	54,54,54,54	0
56	MG	1A	3201	1/1	0.91	0.68	41,41,41,41	0
56	MG	2A	3587	1/1	0.91	0.15	36,36,36,36	0
56	MG	2A	3028	1/1	0.91	0.28	50,50,50,50	0
56	MG	1A	3243	1/1	0.91	0.12	63,63,63,63	0
56	MG	1A	3536	1/1	0.91	0.24	45,45,45,45	0
56	MG	2a	3150	1/1	0.91	0.15	53,53,53,53	0
56	MG	1A	3295	1/1	0.91	0.26	62,62,62,62	0
56	MG	1A	3298	1/1	0.91	0.18	43,43,43,43	0
56	MG	1a	1675	1/1	0.91	0.33	41,41,41,41	0
56	MG	1A	3891	1/1	0.91	0.15	67,67,67,67	0
56	MG	2A	3617	1/1	0.91	0.28	59,59,59,59	0
56	MG	1A	3301	1/1	0.91	1.35	48,48,48,48	0
56	MG	1A	3337	1/1	0.91	0.11	46,46,46,46	0
56	MG	2A	3636	1/1	0.91	0.11	50,50,50,50	0
56	MG	2A	3281	1/1	0.91	1.22	59,59,59,59	0
56	MG	2A	3282	1/1	0.91	0.45	45,45,45,45	0
56	MG	2A	3642	1/1	0.91	0.08	62,62,62,62	0
56	MG	1A	3448	1/1	0.91	0.61	44,44,44,44	0
56	MG	1A	3900	1/1	0.91	0.52	84,84,84,84	0
56	MG	2A	3652	1/1	0.91	0.13	31,31,31,31	0
56	MG	1A	3902	1/1	0.91	0.09	49,49,49,49	0
56	MG	2A	3662	1/1	0.91	0.12	51,51,51,51	0
56	MG	2A	3054	1/1	0.91	0.13	55,55,55,55	0
56	MG	1A	3903	1/1	0.91	0.33	76,76,76,76	0
56	MG	2A	3293	1/1	0.91	0.23	57,57,57,57	0
56	MG	2A	3063	1/1	0.91	0.62	46,46,46,46	0
56	MG	1B	204	1/1	0.91	0.29	49,49,49,49	0
56	MG	2A	3681	1/1	0.91	0.15	63,63,63,63	0
56	MG	2A	3683	1/1	0.91	0.09	44,44,44,44	0
56	MG	1A	3904	1/1	0.91	0.06	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	1B	219	1/1	0.91	0.21	53,53,53,53	0
56	MG	2k	201	1/1	0.91	0.15	59,59,59,59	0
56	MG	2A	3690	1/1	0.91	0.17	43,43,43,43	0
56	MG	2A	3302	1/1	0.91	0.17	46,46,46,46	0
56	MG	1A	3906	1/1	0.91	0.08	67,67,67,67	0
56	MG	2A	3305	1/1	0.91	0.14	60,60,60,60	0
56	MG	1A	3725	1/1	0.91	0.13	36,36,36,36	0
56	MG	2A	3740	1/1	0.92	0.20	71,71,71,71	0
56	MG	2A	3753	1/1	0.92	0.07	69,69,69,69	0
56	MG	1h	201	1/1	0.92	0.09	55,55,55,55	0
56	MG	2A	3765	1/1	0.92	0.07	67,67,67,67	0
56	MG	2A	3189	1/1	0.92	0.12	33,33,33,33	0
56	MG	2A	3771	1/1	0.92	0.14	42,42,42,42	0
56	MG	2A	3394	1/1	0.92	0.70	61,61,61,61	0
56	MG	1A	3703	1/1	0.92	0.17	54,54,54,54	0
56	MG	1A	3387	1/1	0.92	0.28	46,46,46,46	0
56	MG	1a	1632	1/1	0.92	0.26	47,47,47,47	0
56	MG	1A	3065	1/1	0.92	0.12	53,53,53,53	0
56	MG	1A	3109	1/1	0.92	0.23	52,52,52,52	0
56	MG	1A	3876	1/1	0.92	0.14	65,65,65,65	0
56	MG	1A	3204	1/1	0.92	0.14	53,53,53,53	0
56	MG	2A	3804	1/1	0.92	0.15	52,52,52,52	0
56	MG	2B	203	1/1	0.92	0.10	66,66,66,66	0
56	MG	1A	3881	1/1	0.92	0.06	63,63,63,63	0
56	MG	2A	3202	1/1	0.92	0.18	51,51,51,51	0
56	MG	1A	3392	1/1	0.92	1.43	58,58,58,58	0
56	MG	2B	212	1/1	0.92	0.14	61,61,61,61	0
56	MG	1A	3549	1/1	0.92	1.40	46,46,46,46	0
56	MG	2D	303	1/1	0.92	0.53	48,48,48,48	0
56	MG	1A	3888	1/1	0.92	0.13	59,59,59,59	0
56	MG	2A	3438	1/1	0.92	0.26	54,54,54,54	0
56	MG	2E	303	1/1	0.92	0.94	64,64,64,64	0
56	MG	2A	3210	1/1	0.92	0.81	48,48,48,48	0
56	MG	1A	4029	1/1	0.92	0.14	54,54,54,54	0
56	MG	2A	3213	1/1	0.92	0.19	41,41,41,41	0
56	MG	1A	3160	1/1	0.92	0.29	53,53,53,53	0
56	MG	1a	1655	1/1	0.92	0.08	41,41,41,41	0
56	MG	1A	3317	1/1	0.92	0.28	43,43,43,43	0
56	MG	2A	3452	1/1	0.92	0.72	45,45,45,45	0
56	MG	1A	3113	1/1	0.92	0.46	51,51,51,51	0
56	MG	1A	4040	1/1	0.92	0.17	34,34,34,34	0
56	MG	2V	201	1/1	0.92	0.20	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2V	202	1/1	0.92	0.13	38,38,38,38	0
56	MG	1A	3398	1/1	0.92	0.31	56,56,56,56	0
56	MG	2X	101	1/1	0.92	0.14	53,53,53,53	0
56	MG	1A	3174	1/1	0.92	0.32	39,39,39,39	0
56	MG	1A	3255	1/1	0.92	1.06	38,38,38,38	0
56	MG	1A	3740	1/1	0.92	0.26	44,44,44,44	0
56	MG	2A	3463	1/1	0.92	0.15	61,61,61,61	0
56	MG	1A	3045	1/1	0.92	0.61	41,41,41,41	0
56	MG	2A	3465	1/1	0.92	0.13	58,58,58,58	0
56	MG	28	101	1/1	0.92	0.18	47,47,47,47	0
56	MG	2A	3018	1/1	0.92	0.36	56,56,56,56	0
56	MG	1a	1678	1/1	0.92	0.38	60,60,60,60	0
56	MG	1A	3905	1/1	0.92	0.15	44,44,44,44	0
56	MG	1A	3469	1/1	0.92	0.19	33,33,33,33	0
56	MG	1A	3907	1/1	0.92	0.27	39,39,39,39	0
56	MG	2A	3243	1/1	0.92	0.22	60,60,60,60	0
56	MG	1A	3746	1/1	0.92	0.13	51,51,51,51	0
56	MG	2A	3033	1/1	0.92	0.18	35,35,35,35	0
56	MG	2A	3248	1/1	0.92	0.28	53,53,53,53	0
56	MG	2a	3016	1/1	0.92	0.19	61,61,61,61	0
56	MG	1A	3748	1/1	0.92	0.21	59,59,59,59	0
56	MG	2A	3491	1/1	0.92	0.17	42,42,42,42	0
56	MG	1a	1685	1/1	0.92	0.11	42,42,42,42	0
56	MG	1D	309	1/1	0.92	0.38	33,33,33,33	0
56	MG	1a	1690	1/1	0.92	0.71	65,65,65,65	0
56	MG	2A	3501	1/1	0.92	0.13	49,49,49,49	0
56	MG	2A	3503	1/1	0.92	0.43	54,54,54,54	0
56	MG	1A	3068	1/1	0.92	0.21	32,32,32,32	0
56	MG	1A	3060	1/1	0.92	0.18	49,49,49,49	0
56	MG	2A	3515	1/1	0.92	0.13	43,43,43,43	0
56	MG	2A	3518	1/1	0.92	0.09	45,45,45,45	0
56	MG	1A	3751	1/1	0.92	0.16	34,34,34,34	0
56	MG	2a	3036	1/1	0.92	0.13	70,70,70,70	0
56	MG	1E	305	1/1	0.92	1.03	39,39,39,39	0
56	MG	1A	3754	1/1	0.92	1.45	54,54,54,54	0
56	MG	1A	3473	1/1	0.92	0.76	47,47,47,47	0
56	MG	1A	3588	1/1	0.92	0.12	46,46,46,46	0
56	MG	1A	3773	1/1	0.92	0.37	51,51,51,51	0
56	MG	2a	3062	1/1	0.92	0.12	59,59,59,59	0
56	MG	1A	3324	1/1	0.92	0.16	40,40,40,40	0
56	MG	1A	3777	1/1	0.92	0.08	52,52,52,52	0
56	MG	2a	3072	1/1	0.92	0.23	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	3269	1/1	0.92	0.23	50,50,50,50	0
56	MG	1A	3592	1/1	0.92	0.11	79,79,79,79	0
56	MG	2a	3078	1/1	0.92	0.34	58,58,58,58	0
56	MG	1A	3485	1/1	0.92	0.13	33,33,33,33	0
56	MG	1G	204	1/1	0.92	0.12	53,53,53,53	0
56	MG	2A	3560	1/1	0.92	0.51	55,55,55,55	0
56	MG	1A	3787	1/1	0.92	0.12	41,41,41,41	0
56	MG	1A	3597	1/1	0.92	0.22	41,41,41,41	0
56	MG	1A	3326	1/1	0.92	0.23	50,50,50,50	0
56	MG	1R	203	1/1	0.92	0.15	48,48,48,48	0
56	MG	1A	3797	1/1	0.92	0.46	52,52,52,52	0
56	MG	2A	3580	1/1	0.92	0.18	54,54,54,54	0
56	MG	2A	3582	1/1	0.92	0.20	66,66,66,66	0
56	MG	1A	3490	1/1	0.92	0.12	69,69,69,69	0
56	MG	2a	3105	1/1	0.92	0.14	49,49,49,49	0
56	MG	2A	3285	1/1	0.92	0.30	54,54,54,54	0
56	MG	1a	1732	1/1	0.92	0.18	53,53,53,53	0
56	MG	1A	3493	1/1	0.92	0.10	32,32,32,32	0
56	MG	2A	3094	1/1	0.92	0.15	52,52,52,52	0
56	MG	1A	3810	1/1	0.92	0.11	43,43,43,43	0
56	MG	1a	1736	1/1	0.92	0.12	60,60,60,60	0
56	MG	1U	204	1/1	0.92	0.38	40,40,40,40	0
56	MG	1A	3303	1/1	0.92	0.35	38,38,38,38	0
56	MG	1a	1743	1/1	0.92	0.24	44,44,44,44	0
56	MG	2A	3104	1/1	0.92	0.11	39,39,39,39	0
56	MG	1A	3622	1/1	0.92	0.14	37,37,37,37	0
56	MG	2A	3626	1/1	0.92	0.23	75,75,75,75	0
56	MG	2A	3628	1/1	0.92	0.14	57,57,57,57	0
56	MG	1A	3370	1/1	0.92	0.08	48,48,48,48	0
56	MG	2A	3110	1/1	0.92	0.17	40,40,40,40	0
56	MG	1V	204	1/1	0.92	0.21	43,43,43,43	0
56	MG	1W	202	1/1	0.92	0.15	40,40,40,40	0
56	MG	2a	3132	1/1	0.92	0.33	80,80,80,80	0
56	MG	1A	3412	1/1	0.92	0.94	56,56,56,56	0
56	MG	2A	3645	1/1	0.92	0.11	64,64,64,64	0
56	MG	2a	3135	1/1	0.92	0.20	67,67,67,67	0
56	MG	1A	3964	1/1	0.92	0.11	50,50,50,50	0
56	MG	1A	3629	1/1	0.92	0.10	30,30,30,30	0
56	MG	2A	3122	1/1	0.92	0.55	55,55,55,55	0
56	MG	1A	3020	1/1	0.92	0.20	24,24,24,24	0
56	MG	2A	3660	1/1	0.92	0.14	55,55,55,55	0
56	MG	1A	3085	1/1	0.92	0.16	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	10	108	1/1	0.92	0.10	62,62,62,62	0
56	MG	2A	3320	1/1	0.92	0.22	62,62,62,62	0
56	MG	1A	3039	1/1	0.92	0.13	37,37,37,37	0
56	MG	2A	3129	1/1	0.92	0.15	59,59,59,59	0
56	MG	13	103	1/1	0.92	0.20	57,57,57,57	0
56	MG	1A	3198	1/1	0.92	0.21	47,47,47,47	0
56	MG	2A	3325	1/1	0.92	0.16	48,48,48,48	0
56	MG	2A	3146	1/1	0.92	0.15	46,46,46,46	0
56	MG	2a	3173	1/1	0.92	0.10	42,42,42,42	0
56	MG	2A	3331	1/1	0.92	0.76	43,43,43,43	0
56	MG	1a	1778	1/1	0.92	0.12	69,69,69,69	0
56	MG	15	103	1/1	0.92	0.61	37,37,37,37	0
56	MG	1A	3832	1/1	0.92	0.15	42,42,42,42	0
56	MG	2A	3162	1/1	0.92	0.25	54,54,54,54	0
56	MG	1A	3510	1/1	0.92	0.27	53,53,53,53	0
56	MG	2A	3343	1/1	0.92	0.60	54,54,54,54	0
56	MG	1a	1791	1/1	0.92	0.18	59,59,59,59	0
56	MG	1A	3658	1/1	0.92	0.42	43,43,43,43	0
56	MG	1A	3845	1/1	0.92	0.09	62,62,62,62	0
56	MG	2a	3205	1/1	0.92	0.16	36,36,36,36	0
56	MG	1A	3310	1/1	0.92	0.12	48,48,48,48	0
56	MG	1A	3431	1/1	0.92	1.34	66,66,66,66	0
56	MG	1A	3516	1/1	0.92	0.12	44,44,44,44	0
56	MG	2A	3176	1/1	0.92	1.12	65,65,65,65	0
56	MG	1A	3861	1/1	0.92	0.13	55,55,55,55	0
56	MG	1A	3064	1/1	0.92	0.19	43,43,43,43	0
56	MG	1A	3524	1/1	0.92	0.17	36,36,36,36	0
56	MG	1A	3675	1/1	0.92	0.10	57,57,57,57	0
56	MG	1A	3437	1/1	0.92	0.64	41,41,41,41	0
56	MG	2e	201	1/1	0.92	0.13	81,81,81,81	0
56	MG	1a	1617	1/1	0.92	0.50	51,51,51,51	0
56	MG	1b	301	1/1	0.92	0.13	77,77,77,77	0
56	MG	1A	3527	1/1	0.92	0.17	53,53,53,53	0
56	MG	2A	3735	1/1	0.92	0.12	67,67,67,67	0
56	MG	2x	101	1/1	0.92	0.13	61,61,61,61	0
56	MG	2A	3186	1/1	0.92	0.17	40,40,40,40	0
57	ZN	2n	102	1/1	0.92	0.09	98,98,98,98	0
56	MG	1A	3386	1/1	0.92	0.19	37,37,37,37	0
56	MG	1A	3208	1/1	0.93	0.31	59,59,59,59	0
56	MG	1A	3115	1/1	0.93	0.41	41,41,41,41	0
56	MG	2A	3741	1/1	0.93	0.10	68,68,68,68	0
56	MG	2A	3743	1/1	0.93	0.06	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	2A	3746	1/1	0.93	0.10	33,33,33,33	0
56	MG	2A	3750	1/1	0.93	0.09	54,54,54,54	0
56	MG	1A	3262	1/1	0.93	0.54	50,50,50,50	0
56	MG	2A	3393	1/1	0.93	0.23	50,50,50,50	0
56	MG	2A	3764	1/1	0.93	0.20	52,52,52,52	0
56	MG	1A	3058	1/1	0.93	0.20	53,53,53,53	0
56	MG	2A	3395	1/1	0.93	0.08	64,64,64,64	0
56	MG	1A	3176	1/1	0.93	0.26	44,44,44,44	0
56	MG	2A	3397	1/1	0.93	0.07	39,39,39,39	0
56	MG	2A	3402	1/1	0.93	0.42	51,51,51,51	0
56	MG	2A	3779	1/1	0.93	0.15	50,50,50,50	0
56	MG	1A	3475	1/1	0.93	0.11	54,54,54,54	0
56	MG	1A	3726	1/1	0.93	0.11	38,38,38,38	0
56	MG	1A	3727	1/1	0.93	0.09	45,45,45,45	0
56	MG	1a	1621	1/1	0.93	0.27	53,53,53,53	0
56	MG	1A	3884	1/1	0.93	0.23	57,57,57,57	0
56	MG	1A	3585	1/1	0.93	0.15	23,23,23,23	0
56	MG	2A	3799	1/1	0.93	0.34	52,52,52,52	0
56	MG	1a	1627	1/1	0.93	0.19	60,60,60,60	0
56	MG	2A	3418	1/1	0.93	0.16	42,42,42,42	0
56	MG	1a	1628	1/1	0.93	0.15	66,66,66,66	0
56	MG	2A	3427	1/1	0.93	0.19	41,41,41,41	0
56	MG	2A	3196	1/1	0.93	0.57	57,57,57,57	0
56	MG	1a	1631	1/1	0.93	0.23	57,57,57,57	0
56	MG	1A	3406	1/1	0.93	0.82	55,55,55,55	0
56	MG	2A	3437	1/1	0.93	0.17	30,30,30,30	0
56	MG	1A	4026	1/1	0.93	0.15	66,66,66,66	0
56	MG	2A	3439	1/1	0.93	0.32	62,62,62,62	0
56	MG	1A	3179	1/1	0.93	0.10	35,35,35,35	0
56	MG	1a	1637	1/1	0.93	0.21	48,48,48,48	0
56	MG	1A	3889	1/1	0.93	0.14	33,33,33,33	0
56	MG	2A	3205	1/1	0.93	0.54	52,52,52,52	0
56	MG	1A	3217	1/1	0.93	0.10	68,68,68,68	0
56	MG	1x	105	1/1	0.93	0.12	57,57,57,57	0
56	MG	2Q	201	1/1	0.93	0.17	56,56,56,56	0
56	MG	1A	3059	1/1	0.93	0.08	55,55,55,55	0
56	MG	1A	3277	1/1	0.93	0.38	37,37,37,37	0
56	MG	1A	3898	1/1	0.93	0.11	46,46,46,46	0
56	MG	1A	3745	1/1	0.93	0.17	46,46,46,46	0
56	MG	2T	202	1/1	0.93	0.22	62,62,62,62	0
56	MG	1a	1648	1/1	0.93	0.22	50,50,50,50	0
56	MG	1A	3224	1/1	0.93	1.10	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	2W	201	1/1	0.93	0.78	44,44,44,44	0
56	MG	1B	203	1/1	0.93	0.24	47,47,47,47	0
56	MG	1A	3416	1/1	0.93	0.27	36,36,36,36	0
56	MG	1A	3418	1/1	0.93	0.68	46,46,46,46	0
56	MG	2A	3226	1/1	0.93	0.26	49,49,49,49	0
56	MG	1B	214	1/1	0.93	0.08	52,52,52,52	0
56	MG	1B	217	1/1	0.93	0.16	37,37,37,37	0
56	MG	2A	3230	1/1	0.93	0.11	47,47,47,47	0
56	MG	1A	3006	1/1	0.93	0.37	35,35,35,35	0
56	MG	1A	3615	1/1	0.93	0.14	30,30,30,30	0
56	MG	2A	3236	1/1	0.93	0.44	52,52,52,52	0
56	MG	2A	3477	1/1	0.93	0.12	47,47,47,47	0
56	MG	1A	3616	1/1	0.93	0.17	26,26,26,26	0
56	MG	1a	1670	1/1	0.93	0.14	60,60,60,60	0
56	MG	1A	3619	1/1	0.93	0.17	43,43,43,43	0
56	MG	1a	1673	1/1	0.93	0.13	43,43,43,43	0
56	MG	2A	3027	1/1	0.93	0.48	61,61,61,61	0
56	MG	1a	1674	1/1	0.93	0.23	37,37,37,37	0
56	MG	2A	3029	1/1	0.93	0.25	54,54,54,54	0
56	MG	2A	3495	1/1	0.93	0.09	61,61,61,61	0
56	MG	2A	3498	1/1	0.93	0.20	51,51,51,51	0
56	MG	2A	3246	1/1	0.93	0.11	44,44,44,44	0
56	MG	1A	3422	1/1	0.93	0.51	46,46,46,46	0
56	MG	1A	3912	1/1	0.93	0.16	44,44,44,44	0
56	MG	1A	3040	1/1	0.93	0.36	37,37,37,37	0
56	MG	2A	3509	1/1	0.93	0.13	46,46,46,46	0
56	MG	1D	301	1/1	0.93	0.32	44,44,44,44	0
56	MG	1A	3288	1/1	0.93	0.19	37,37,37,37	0
56	MG	2A	3038	1/1	0.93	0.14	44,44,44,44	0
56	MG	2A	3039	1/1	0.93	0.23	53,53,53,53	0
56	MG	1A	3920	1/1	0.93	0.17	31,31,31,31	0
56	MG	1A	3375	1/1	0.93	0.23	57,57,57,57	0
56	MG	2A	3259	1/1	0.93	0.08	54,54,54,54	0
56	MG	2a	3037	1/1	0.93	0.08	66,66,66,66	0
56	MG	2a	3038	1/1	0.93	0.21	41,41,41,41	0
56	MG	2a	3040	1/1	0.93	0.49	65,65,65,65	0
56	MG	2a	3042	1/1	0.93	1.06	51,51,51,51	0
56	MG	1A	3190	1/1	0.93	0.23	32,32,32,32	0
56	MG	2a	3047	1/1	0.93	0.18	55,55,55,55	0
56	MG	2A	3536	1/1	0.93	0.23	56,56,56,56	0
56	MG	1A	3781	1/1	0.93	1.18	61,61,61,61	0
56	MG	2a	3054	1/1	0.93	0.21	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	3048	1/1	0.93	0.13	50,50,50,50	0
56	MG	2a	3060	1/1	0.93	0.12	78,78,78,78	0
56	MG	2A	3541	1/1	0.93	0.12	46,46,46,46	0
56	MG	1A	3030	1/1	0.93	0.19	49,49,49,49	0
56	MG	2a	3066	1/1	0.93	0.07	43,43,43,43	0
56	MG	2a	3067	1/1	0.93	0.12	49,49,49,49	0
56	MG	1A	3053	1/1	0.93	0.11	34,34,34,34	0
56	MG	2A	3052	1/1	0.93	0.09	61,61,61,61	0
56	MG	1A	3639	1/1	0.93	0.12	24,24,24,24	0
56	MG	1a	1694	1/1	0.93	0.48	51,51,51,51	0
56	MG	2A	3057	1/1	0.93	0.28	45,45,45,45	0
56	MG	2A	3275	1/1	0.93	0.75	58,58,58,58	0
56	MG	1A	3929	1/1	0.93	0.16	26,26,26,26	0
56	MG	1A	3642	1/1	0.93	0.20	36,36,36,36	0
56	MG	1A	3098	1/1	0.93	0.12	46,46,46,46	0
56	MG	1A	3934	1/1	0.93	0.10	49,49,49,49	0
56	MG	1A	3056	1/1	0.93	0.19	32,32,32,32	0
56	MG	1A	3649	1/1	0.93	0.15	31,31,31,31	0
56	MG	2a	3092	1/1	0.93	0.39	60,60,60,60	0
56	MG	1A	3107	1/1	0.93	0.54	48,48,48,48	0
56	MG	1A	3654	1/1	0.93	0.16	31,31,31,31	0
56	MG	1A	3332	1/1	0.93	0.22	45,45,45,45	0
56	MG	2a	3101	1/1	0.93	0.22	62,62,62,62	0
56	MG	2A	3079	1/1	0.93	0.19	52,52,52,52	0
56	MG	1Q	205	1/1	0.93	0.34	36,36,36,36	0
56	MG	1R	201	1/1	0.93	0.31	45,45,45,45	0
56	MG	2A	3596	1/1	0.93	0.07	32,32,32,32	0
56	MG	1A	3659	1/1	0.93	0.16	53,53,53,53	0
56	MG	2A	3600	1/1	0.93	0.18	53,53,53,53	0
56	MG	2a	3110	1/1	0.93	0.21	53,53,53,53	0
56	MG	1A	3299	1/1	0.93	0.25	49,49,49,49	0
56	MG	2A	3612	1/1	0.93	0.33	49,49,49,49	0
56	MG	2A	3614	1/1	0.93	0.24	66,66,66,66	0
56	MG	2A	3087	1/1	0.93	0.63	54,54,54,54	0
56	MG	2A	3088	1/1	0.93	0.20	49,49,49,49	0
56	MG	1a	1724	1/1	0.93	0.14	47,47,47,47	0
56	MG	1A	3943	1/1	0.93	0.15	64,64,64,64	0
56	MG	1A	3945	1/1	0.93	0.13	35,35,35,35	0
56	MG	1A	3334	1/1	0.93	0.20	53,53,53,53	0
56	MG	2a	3121	1/1	0.93	0.18	63,63,63,63	0
56	MG	2a	3122	1/1	0.93	0.10	63,63,63,63	0
56	MG	1U	203	1/1	0.93	0.61	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	3635	1/1	0.93	0.58	76,76,76,76	0
56	MG	1A	3300	1/1	0.93	0.53	27,27,27,27	0
56	MG	1A	3663	1/1	0.93	0.12	32,32,32,32	0
56	MG	2A	3639	1/1	0.93	0.06	59,59,59,59	0
56	MG	1U	208	1/1	0.93	1.06	40,40,40,40	0
56	MG	1A	3450	1/1	0.93	0.28	53,53,53,53	0
56	MG	2A	3310	1/1	0.93	0.09	55,55,55,55	0
56	MG	2A	3311	1/1	0.93	0.49	43,43,43,43	0
56	MG	1A	3159	1/1	0.93	0.35	60,60,60,60	0
56	MG	1A	3251	1/1	0.93	0.22	39,39,39,39	0
56	MG	2A	3653	1/1	0.93	0.09	56,56,56,56	0
56	MG	2a	3140	1/1	0.93	0.16	61,61,61,61	0
56	MG	1V	206	1/1	0.93	0.18	47,47,47,47	0
56	MG	1A	3057	1/1	0.93	0.16	59,59,59,59	0
56	MG	1a	1750	1/1	0.93	0.28	49,49,49,49	0
56	MG	2A	3665	1/1	0.93	0.16	57,57,57,57	0
56	MG	1X	101	1/1	0.93	0.69	43,43,43,43	0
56	MG	2A	3118	1/1	0.93	0.28	58,58,58,58	0
56	MG	2a	3153	1/1	0.93	0.05	76,76,76,76	0
56	MG	2A	3120	1/1	0.93	0.10	66,66,66,66	0
56	MG	1a	1757	1/1	0.93	0.15	65,65,65,65	0
56	MG	2A	3676	1/1	0.93	0.20	45,45,45,45	0
56	MG	2a	3164	1/1	0.93	0.40	70,70,70,70	0
56	MG	2A	3677	1/1	0.93	0.10	66,66,66,66	0
56	MG	2a	3170	1/1	0.93	0.19	60,60,60,60	0
56	MG	1a	1760	1/1	0.93	0.07	55,55,55,55	0
56	MG	2a	3172	1/1	0.93	0.11	39,39,39,39	0
56	MG	1A	3840	1/1	0.93	0.36	69,69,69,69	0
56	MG	1A	3552	1/1	0.93	0.15	40,40,40,40	0
56	MG	1A	3691	1/1	0.93	0.16	28,28,28,28	0
56	MG	10	102	1/1	0.93	0.32	68,68,68,68	0
56	MG	1A	3848	1/1	0.93	0.26	43,43,43,43	0
56	MG	2A	3134	1/1	0.93	0.23	61,61,61,61	0
56	MG	2a	3188	1/1	0.93	0.07	58,58,58,58	0
56	MG	2a	3189	1/1	0.93	0.13	72,72,72,72	0
56	MG	2a	3190	1/1	0.93	0.20	61,61,61,61	0
56	MG	1A	3851	1/1	0.93	0.20	48,48,48,48	0
56	MG	1A	3852	1/1	0.93	0.15	36,36,36,36	0
56	MG	2A	3144	1/1	0.93	0.70	48,48,48,48	0
56	MG	1A	3692	1/1	0.93	0.75	36,36,36,36	0
56	MG	2A	3702	1/1	0.93	0.15	50,50,50,50	0
56	MG	2A	3705	1/1	0.93	0.15	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	3707	1/1	0.93	0.19	63,63,63,63	0
56	MG	1A	3979	1/1	0.93	0.08	50,50,50,50	0
56	MG	1A	3456	1/1	0.93	0.23	40,40,40,40	0
56	MG	1a	1775	1/1	0.93	0.20	56,56,56,56	0
56	MG	1A	3702	1/1	0.93	0.08	55,55,55,55	0
56	MG	1A	3860	1/1	0.93	0.20	37,37,37,37	0
56	MG	1A	3556	1/1	0.93	0.11	50,50,50,50	0
56	MG	1a	1781	1/1	0.93	0.09	49,49,49,49	0
56	MG	1A	3067	1/1	0.93	0.15	34,34,34,34	0
56	MG	17	106	1/1	0.93	0.93	41,41,41,41	0
56	MG	1a	1789	1/1	0.93	0.06	61,61,61,61	0
56	MG	2A	3364	1/1	0.93	0.15	80,80,80,80	0
56	MG	1A	3710	1/1	0.93	0.12	46,46,46,46	0
56	MG	18	101	1/1	0.93	1.59	53,53,53,53	0
56	MG	2A	3378	1/1	0.93	0.15	47,47,47,47	0
56	MG	1A	3711	1/1	0.93	0.11	25,25,25,25	0
57	ZN	24	501	1/1	0.93	0.07	114,114,114,114	0
56	MG	1A	3343	1/1	0.93	0.15	45,45,45,45	0
56	MG	1A	3207	1/1	0.93	0.51	47,47,47,47	0
56	MG	2A	3680	1/1	0.94	0.14	58,58,58,58	0
56	MG	1A	3700	1/1	0.94	0.07	55,55,55,55	0
56	MG	1A	3701	1/1	0.94	0.15	39,39,39,39	0
56	MG	1A	3049	1/1	0.94	0.21	39,39,39,39	0
56	MG	2A	3301	1/1	0.94	0.40	57,57,57,57	0
56	MG	2A	3045	1/1	0.94	0.42	52,52,52,52	0
56	MG	1a	1646	1/1	0.94	0.41	48,48,48,48	0
56	MG	1A	4021	1/1	0.94	0.18	64,64,64,64	0
56	MG	1a	1652	1/1	0.94	0.07	54,54,54,54	0
56	MG	1A	3038	1/1	0.94	0.20	55,55,55,55	0
56	MG	1A	4023	1/1	0.94	0.41	57,57,57,57	0
56	MG	1A	3228	1/1	0.94	0.39	57,57,57,57	0
56	MG	2A	3704	1/1	0.94	0.36	57,57,57,57	0
56	MG	1a	1659	1/1	0.94	0.22	62,62,62,62	0
56	MG	1A	3559	1/1	0.94	0.13	34,34,34,34	0
56	MG	2A	3056	1/1	0.94	0.12	67,67,67,67	0
56	MG	1a	1661	1/1	0.94	0.92	70,70,70,70	0
56	MG	1A	3458	1/1	0.94	0.10	63,63,63,63	0
56	MG	2A	3061	1/1	0.94	0.14	37,37,37,37	0
56	MG	2A	3715	1/1	0.94	0.34	63,63,63,63	0
56	MG	1A	3463	1/1	0.94	0.21	56,56,56,56	0
56	MG	1A	3002	1/1	0.94	0.08	52,52,52,52	0
56	MG	1A	3075	1/1	0.94	0.23	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	1668	1/1	0.94	0.16	70,70,70,70	0
56	MG	1A	3567	1/1	0.94	0.18	36,36,36,36	0
56	MG	1A	4036	1/1	0.94	0.14	40,40,40,40	0
56	MG	2A	3072	1/1	0.94	0.28	51,51,51,51	0
56	MG	2A	3728	1/1	0.94	0.22	64,64,64,64	0
56	MG	1A	3719	1/1	0.94	0.11	60,60,60,60	0
56	MG	2A	3329	1/1	0.94	0.55	55,55,55,55	0
56	MG	1a	1672	1/1	0.94	0.09	56,56,56,56	0
56	MG	2A	3076	1/1	0.94	0.58	56,56,56,56	0
56	MG	1A	3568	1/1	0.94	0.21	39,39,39,39	0
56	MG	2A	3335	1/1	0.94	0.14	52,52,52,52	0
56	MG	2A	3737	1/1	0.94	0.10	54,54,54,54	0
56	MG	1A	3575	1/1	0.94	0.16	57,57,57,57	0
56	MG	2A	3340	1/1	0.94	0.10	69,69,69,69	0
56	MG	1B	202	1/1	0.94	0.16	46,46,46,46	0
56	MG	2A	3083	1/1	0.94	0.09	46,46,46,46	0
56	MG	2A	3744	1/1	0.94	0.15	59,59,59,59	0
56	MG	2A	3745	1/1	0.94	0.11	45,45,45,45	0
56	MG	2A	3084	1/1	0.94	0.20	35,35,35,35	0
56	MG	2A	3747	1/1	0.94	0.09	58,58,58,58	0
56	MG	1A	3279	1/1	0.94	0.36	41,41,41,41	0
56	MG	1A	3315	1/1	0.94	0.17	34,34,34,34	0
56	MG	2A	3349	1/1	0.94	0.16	58,58,58,58	0
56	MG	2A	3755	1/1	0.94	0.25	62,62,62,62	0
56	MG	2A	3759	1/1	0.94	0.12	33,33,33,33	0
56	MG	2A	3760	1/1	0.94	0.07	65,65,65,65	0
56	MG	2A	3763	1/1	0.94	0.32	65,65,65,65	0
56	MG	1B	205	1/1	0.94	0.28	50,50,50,50	0
56	MG	1B	206	1/1	0.94	0.14	55,55,55,55	0
56	MG	1B	208	1/1	0.94	0.14	50,50,50,50	0
56	MG	2A	3770	1/1	0.94	0.08	60,60,60,60	0
56	MG	2A	3093	1/1	0.94	0.33	63,63,63,63	0
56	MG	2A	3357	1/1	0.94	1.14	67,67,67,67	0
56	MG	2A	3775	1/1	0.94	0.17	51,51,51,51	0
56	MG	1A	3023	1/1	0.94	0.39	47,47,47,47	0
56	MG	1A	3157	1/1	0.94	0.13	39,39,39,39	0
56	MG	1A	3236	1/1	0.94	0.49	57,57,57,57	0
56	MG	2A	3784	1/1	0.94	0.13	58,58,58,58	0
56	MG	1a	1687	1/1	0.94	0.24	49,49,49,49	0
56	MG	1a	1689	1/1	0.94	0.15	55,55,55,55	0
56	MG	1A	3890	1/1	0.94	0.19	49,49,49,49	0
56	MG	1A	3200	1/1	0.94	0.31	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	1B	223	1/1	0.94	0.20	58,58,58,58	0
56	MG	2A	3797	1/1	0.94	0.15	42,42,42,42	0
56	MG	2A	3372	1/1	0.94	0.14	63,63,63,63	0
56	MG	2A	3377	1/1	0.94	0.21	41,41,41,41	0
56	MG	2A	3806	1/1	0.94	0.11	51,51,51,51	0
56	MG	2A	3108	1/1	0.94	0.40	50,50,50,50	0
56	MG	1a	1693	1/1	0.94	0.50	58,58,58,58	0
56	MG	2A	3382	1/1	0.94	0.11	41,41,41,41	0
56	MG	1A	3892	1/1	0.94	0.14	63,63,63,63	0
56	MG	2B	209	1/1	0.94	0.17	70,70,70,70	0
56	MG	1A	3363	1/1	0.94	0.18	43,43,43,43	0
56	MG	1A	3484	1/1	0.94	0.78	39,39,39,39	0
56	MG	2D	301	1/1	0.94	0.36	39,39,39,39	0
56	MG	2A	3113	1/1	0.94	0.12	66,66,66,66	0
56	MG	2D	304	1/1	0.94	0.38	54,54,54,54	0
56	MG	2A	3391	1/1	0.94	0.12	54,54,54,54	0
56	MG	1a	1701	1/1	0.94	0.37	55,55,55,55	0
56	MG	1A	3741	1/1	0.94	0.12	35,35,35,35	0
56	MG	1A	3054	1/1	0.94	0.15	30,30,30,30	0
56	MG	1A	3413	1/1	0.94	0.98	42,42,42,42	0
56	MG	1D	305	1/1	0.94	0.19	44,44,44,44	0
56	MG	1A	3901	1/1	0.94	0.11	63,63,63,63	0
56	MG	2A	3400	1/1	0.94	0.14	60,60,60,60	0
56	MG	2A	3401	1/1	0.94	0.09	49,49,49,49	0
56	MG	1A	3488	1/1	0.94	0.58	49,49,49,49	0
56	MG	2A	3405	1/1	0.94	0.14	43,43,43,43	0
56	MG	1A	3415	1/1	0.94	0.09	58,58,58,58	0
56	MG	1A	3747	1/1	0.94	0.19	56,56,56,56	0
56	MG	1A	3018	1/1	0.94	0.14	53,53,53,53	0
56	MG	2T	204	1/1	0.94	0.14	47,47,47,47	0
56	MG	1E	306	1/1	0.94	0.23	33,33,33,33	0
56	MG	1A	3494	1/1	0.94	0.57	36,36,36,36	0
56	MG	2A	3136	1/1	0.94	0.22	43,43,43,43	0
56	MG	2A	3138	1/1	0.94	0.07	65,65,65,65	0
56	MG	2A	3139	1/1	0.94	0.13	53,53,53,53	0
56	MG	2A	3140	1/1	0.94	0.17	61,61,61,61	0
56	MG	2A	3422	1/1	0.94	0.25	65,65,65,65	0
56	MG	1A	3610	1/1	0.94	0.09	32,32,32,32	0
56	MG	1F	301	1/1	0.94	0.48	40,40,40,40	0
56	MG	2A	3431	1/1	0.94	0.15	51,51,51,51	0
56	MG	2A	3434	1/1	0.94	0.17	54,54,54,54	0
56	MG	1A	3417	1/1	0.94	0.83	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	3001	1/1	0.94	0.25	52,52,52,52	0
56	MG	1A	3367	1/1	0.94	1.05	44,44,44,44	0
56	MG	2A	3147	1/1	0.94	0.16	65,65,65,65	0
56	MG	2A	3151	1/1	0.94	0.10	50,50,50,50	0
56	MG	1A	3913	1/1	0.94	0.18	47,47,47,47	0
56	MG	1F	306	1/1	0.94	0.83	31,31,31,31	0
56	MG	1A	3916	1/1	0.94	0.24	80,80,80,80	0
56	MG	1F	309	1/1	0.94	0.75	52,52,52,52	0
56	MG	1A	3291	1/1	0.94	0.91	46,46,46,46	0
56	MG	2A	3446	1/1	0.94	0.21	36,36,36,36	0
56	MG	1A	3757	1/1	0.94	0.15	41,41,41,41	0
56	MG	1A	3919	1/1	0.94	0.31	56,56,56,56	0
56	MG	1A	3759	1/1	0.94	0.19	48,48,48,48	0
56	MG	1a	1746	1/1	0.94	0.11	44,44,44,44	0
56	MG	1A	3620	1/1	0.94	0.10	36,36,36,36	0
56	MG	1a	1749	1/1	0.94	0.24	63,63,63,63	0
56	MG	2A	3456	1/1	0.94	0.68	59,59,59,59	0
56	MG	2A	3174	1/1	0.94	0.14	55,55,55,55	0
56	MG	1Q	201	1/1	0.94	0.09	44,44,44,44	0
56	MG	1A	3769	1/1	0.94	0.45	47,47,47,47	0
56	MG	1Q	204	1/1	0.94	0.15	20,20,20,20	0
56	MG	1a	1759	1/1	0.94	0.10	45,45,45,45	0
56	MG	2a	3034	1/1	0.94	0.14	55,55,55,55	0
56	MG	1A	3241	1/1	0.94	0.41	39,39,39,39	0
56	MG	2A	3466	1/1	0.94	0.20	44,44,44,44	0
56	MG	1A	3774	1/1	0.94	0.61	54,54,54,54	0
56	MG	1A	3500	1/1	0.94	0.16	29,29,29,29	0
56	MG	2a	3039	1/1	0.94	0.14	47,47,47,47	0
56	MG	2A	3471	1/1	0.94	0.21	53,53,53,53	0
56	MG	1S	202	1/1	0.94	0.20	35,35,35,35	0
56	MG	2a	3043	1/1	0.94	0.21	68,68,68,68	0
56	MG	1A	3502	1/1	0.94	0.24	37,37,37,37	0
56	MG	2a	3045	1/1	0.94	0.59	47,47,47,47	0
56	MG	2a	3046	1/1	0.94	0.20	72,72,72,72	0
56	MG	1T	202	1/1	0.94	0.44	49,49,49,49	0
56	MG	1A	3162	1/1	0.94	1.34	52,52,52,52	0
56	MG	1A	3930	1/1	0.94	0.09	39,39,39,39	0
56	MG	2A	3482	1/1	0.94	0.17	49,49,49,49	0
56	MG	2a	3055	1/1	0.94	0.43	64,64,64,64	0
56	MG	1A	3931	1/1	0.94	0.12	34,34,34,34	0
56	MG	1A	3505	1/1	0.94	0.17	38,38,38,38	0
56	MG	2A	3485	1/1	0.94	0.14	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3191	1/1	0.94	0.23	51,51,51,51	0
56	MG	2A	3488	1/1	0.94	0.18	40,40,40,40	0
56	MG	1A	3783	1/1	0.94	0.15	57,57,57,57	0
56	MG	1A	3784	1/1	0.94	0.15	59,59,59,59	0
56	MG	1U	207	1/1	0.94	0.70	38,38,38,38	0
56	MG	1A	3632	1/1	0.94	0.20	51,51,51,51	0
56	MG	1A	3424	1/1	0.94	0.14	31,31,31,31	0
56	MG	2a	3076	1/1	0.94	0.36	56,56,56,56	0
56	MG	2A	3497	1/1	0.94	0.55	58,58,58,58	0
56	MG	1A	3788	1/1	0.94	0.14	43,43,43,43	0
56	MG	1a	1785	1/1	0.94	0.10	68,68,68,68	0
56	MG	1A	3637	1/1	0.94	0.14	29,29,29,29	0
56	MG	1A	3009	1/1	0.94	0.27	51,51,51,51	0
56	MG	2A	3504	1/1	0.94	0.10	47,47,47,47	0
56	MG	2A	3506	1/1	0.94	0.14	48,48,48,48	0
56	MG	1A	3791	1/1	0.94	0.09	56,56,56,56	0
56	MG	1a	1790	1/1	0.94	0.25	51,51,51,51	0
56	MG	2a	3093	1/1	0.94	0.69	53,53,53,53	0
56	MG	1A	3794	1/1	0.94	0.09	51,51,51,51	0
56	MG	2A	3514	1/1	0.94	0.08	61,61,61,61	0
56	MG	1A	3795	1/1	0.94	0.09	51,51,51,51	0
56	MG	2A	3516	1/1	0.94	0.09	65,65,65,65	0
56	MG	1A	3297	1/1	0.94	0.15	44,44,44,44	0
56	MG	2A	3520	1/1	0.94	0.06	44,44,44,44	0
56	MG	1Z	301	1/1	0.94	0.18	32,32,32,32	0
56	MG	2A	3524	1/1	0.94	0.45	61,61,61,61	0
56	MG	2A	3212	1/1	0.94	0.92	47,47,47,47	0
56	MG	1Z	302	1/1	0.94	0.17	42,42,42,42	0
56	MG	1A	3513	1/1	0.94	0.48	38,38,38,38	0
56	MG	2A	3528	1/1	0.94	0.18	54,54,54,54	0
56	MG	2A	3531	1/1	0.94	0.10	35,35,35,35	0
56	MG	1A	3950	1/1	0.94	0.21	82,82,82,82	0
56	MG	2A	3535	1/1	0.94	0.43	59,59,59,59	0
56	MG	10	103	1/1	0.94	0.50	39,39,39,39	0
56	MG	1a	1809	1/1	0.94	0.06	48,48,48,48	0
56	MG	1A	3951	1/1	0.94	0.07	50,50,50,50	0
56	MG	1A	3953	1/1	0.94	0.12	39,39,39,39	0
56	MG	1a	1815	1/1	0.94	0.07	60,60,60,60	0
56	MG	10	107	1/1	0.94	0.25	30,30,30,30	0
56	MG	2A	3551	1/1	0.94	0.10	41,41,41,41	0
56	MG	1A	3802	1/1	0.94	0.12	33,33,33,33	0
56	MG	1A	3955	1/1	0.94	0.23	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	3803	1/1	0.94	0.14	55,55,55,55	0
56	MG	1A	3168	1/1	0.94	0.12	37,37,37,37	0
56	MG	1A	3959	1/1	0.94	0.09	48,48,48,48	0
56	MG	2a	3131	1/1	0.94	0.09	73,73,73,73	0
56	MG	1A	3091	1/1	0.94	0.20	60,60,60,60	0
56	MG	1A	3253	1/1	0.94	0.69	46,46,46,46	0
56	MG	1A	3435	1/1	0.94	0.22	61,61,61,61	0
56	MG	2A	3240	1/1	0.94	0.12	49,49,49,49	0
56	MG	1A	3520	1/1	0.94	0.60	36,36,36,36	0
56	MG	1A	3966	1/1	0.94	0.08	46,46,46,46	0
56	MG	2A	3583	1/1	0.94	0.17	56,56,56,56	0
56	MG	2a	3139	1/1	0.94	0.14	75,75,75,75	0
56	MG	1A	3822	1/1	0.94	0.49	38,38,38,38	0
56	MG	18	103	1/1	0.94	0.15	33,33,33,33	0
56	MG	19	101	1/1	0.94	0.72	52,52,52,52	0
56	MG	2a	3143	1/1	0.94	0.12	57,57,57,57	0
56	MG	1x	101	1/1	0.94	0.20	42,42,42,42	0
56	MG	1A	3209	1/1	0.94	0.81	51,51,51,51	0
56	MG	2a	3149	1/1	0.94	0.14	67,67,67,67	0
56	MG	1A	3092	1/1	0.94	0.11	49,49,49,49	0
56	MG	1A	3388	1/1	0.94	0.14	51,51,51,51	0
56	MG	1A	3529	1/1	0.94	0.72	36,36,36,36	0
56	MG	1A	3976	1/1	0.94	0.11	67,67,67,67	0
56	MG	1A	3977	1/1	0.94	0.12	43,43,43,43	0
56	MG	2a	3157	1/1	0.94	0.18	58,58,58,58	0
56	MG	2A	3607	1/1	0.94	0.20	35,35,35,35	0
56	MG	2a	3159	1/1	0.94	0.24	59,59,59,59	0
56	MG	2A	3608	1/1	0.94	0.18	64,64,64,64	0
56	MG	1A	3442	1/1	0.94	0.47	49,49,49,49	0
56	MG	2a	3166	1/1	0.94	0.14	41,41,41,41	0
56	MG	2a	3168	1/1	0.94	0.25	74,74,74,74	0
56	MG	2a	3169	1/1	0.94	0.51	65,65,65,65	0
56	MG	1A	3122	1/1	0.94	0.39	53,53,53,53	0
56	MG	1x	115	1/1	0.94	0.19	71,71,71,71	0
56	MG	1A	3664	1/1	0.94	0.40	69,69,69,69	0
56	MG	1A	3666	1/1	0.94	0.17	53,53,53,53	0
56	MG	2A	3619	1/1	0.94	0.11	45,45,45,45	0
56	MG	2a	3176	1/1	0.94	0.25	67,67,67,67	0
56	MG	2a	3177	1/1	0.94	0.13	71,71,71,71	0
56	MG	2A	3621	1/1	0.94	0.18	42,42,42,42	0
56	MG	2A	3262	1/1	0.94	0.34	46,46,46,46	0
56	MG	2A	3003	1/1	0.94	0.18	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	3184	1/1	0.94	0.11	69,69,69,69	0
56	MG	2A	3627	1/1	0.94	0.20	55,55,55,55	0
56	MG	2A	3005	1/1	0.94	0.12	71,71,71,71	0
56	MG	2A	3632	1/1	0.94	0.13	60,60,60,60	0
56	MG	1A	3839	1/1	0.94	0.12	34,34,34,34	0
56	MG	1A	3986	1/1	0.94	0.12	45,45,45,45	0
56	MG	1A	3094	1/1	0.94	0.21	33,33,33,33	0
56	MG	2A	3011	1/1	0.94	0.28	52,52,52,52	0
56	MG	2a	3195	1/1	0.94	0.12	52,52,52,52	0
56	MG	2A	3012	1/1	0.94	0.38	64,64,64,64	0
56	MG	2a	3198	1/1	0.94	0.10	62,62,62,62	0
56	MG	1A	3128	1/1	0.94	0.31	25,25,25,25	0
56	MG	2A	3641	1/1	0.94	0.31	58,58,58,58	0
56	MG	1a	1626	1/1	0.94	0.13	66,66,66,66	0
56	MG	2A	3016	1/1	0.94	0.54	57,57,57,57	0
56	MG	1A	3538	1/1	0.94	0.13	28,28,28,28	0
56	MG	1A	3341	1/1	0.94	0.26	50,50,50,50	0
56	MG	2A	3650	1/1	0.94	0.16	62,62,62,62	0
56	MG	1a	1630	1/1	0.94	0.27	57,57,57,57	0
56	MG	1A	3849	1/1	0.94	0.18	45,45,45,45	0
56	MG	1A	3394	1/1	0.94	0.16	57,57,57,57	0
56	MG	2A	3659	1/1	0.94	0.13	36,36,36,36	0
56	MG	1A	3546	1/1	0.94	0.46	49,49,49,49	0
56	MG	2i	201	1/1	0.94	0.09	54,54,54,54	0
56	MG	1a	1635	1/1	0.94	0.21	43,43,43,43	0
56	MG	2l	201	1/1	0.94	0.14	51,51,51,51	0
56	MG	1A	3307	1/1	0.94	0.46	55,55,55,55	0
56	MG	2A	3288	1/1	0.94	0.98	44,44,44,44	0
56	MG	2A	3289	1/1	0.94	0.34	49,49,49,49	0
56	MG	1A	3855	1/1	0.94	0.13	60,60,60,60	0
56	MG	1A	3693	1/1	0.94	0.13	31,31,31,31	0
56	MG	2x	104	1/1	0.94	0.20	50,50,50,50	0
57	ZN	14	501	1/1	0.94	0.14	90,90,90,90	0
56	MG	1A	3694	1/1	0.94	0.19	70,70,70,70	0
56	MG	1a	1640	1/1	0.94	0.17	59,59,59,59	0
56	MG	1A	3129	1/1	0.94	0.19	47,47,47,47	0
56	MG	1A	3634	1/1	0.95	0.23	65,65,65,65	0
56	MG	2A	3802	1/1	0.95	0.36	60,60,60,60	0
56	MG	1a	1734	1/1	0.95	0.42	61,61,61,61	0
56	MG	1A	3635	1/1	0.95	0.11	43,43,43,43	0
56	MG	2A	3807	1/1	0.95	0.12	51,51,51,51	0
56	MG	2A	3811	1/1	0.95	0.29	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3070	1/1	0.95	0.13	38,38,38,38	0
56	MG	1A	3885	1/1	0.95	0.09	58,58,58,58	0
56	MG	2B	205	1/1	0.95	0.09	62,62,62,62	0
56	MG	1A	3539	1/1	0.95	0.16	43,43,43,43	0
56	MG	1A	3474	1/1	0.95	0.56	40,40,40,40	0
56	MG	1A	3542	1/1	0.95	0.77	46,46,46,46	0
56	MG	2B	211	1/1	0.95	0.15	51,51,51,51	0
56	MG	1A	3758	1/1	0.95	0.13	48,48,48,48	0
56	MG	2B	213	1/1	0.95	0.28	46,46,46,46	0
56	MG	17	102	1/1	0.95	0.25	34,34,34,34	0
56	MG	2A	3502	1/1	0.95	0.15	58,58,58,58	0
56	MG	1a	1748	1/1	0.95	0.95	55,55,55,55	0
56	MG	2A	3081	1/1	0.95	0.17	62,62,62,62	0
56	MG	1A	3543	1/1	0.95	0.13	33,33,33,33	0
56	MG	2A	3507	1/1	0.95	0.12	44,44,44,44	0
56	MG	1A	3640	1/1	0.95	0.15	37,37,37,37	0
56	MG	1A	3763	1/1	0.95	0.10	48,48,48,48	0
56	MG	2A	3510	1/1	0.95	0.10	44,44,44,44	0
56	MG	1a	1752	1/1	0.95	0.17	65,65,65,65	0
56	MG	2A	3513	1/1	0.95	0.10	70,70,70,70	0
56	MG	2G	201	1/1	0.95	0.14	52,52,52,52	0
56	MG	2A	3283	1/1	0.95	0.47	60,60,60,60	0
56	MG	1a	1753	1/1	0.95	0.20	58,58,58,58	0
56	MG	1a	1756	1/1	0.95	0.20	70,70,70,70	0
56	MG	1A	3768	1/1	0.95	0.15	38,38,38,38	0
56	MG	1A	3247	1/1	0.95	0.99	41,41,41,41	0
56	MG	1A	3770	1/1	0.95	0.50	63,63,63,63	0
56	MG	19	102	1/1	0.95	0.68	45,45,45,45	0
56	MG	1A	3193	1/1	0.95	0.16	58,58,58,58	0
56	MG	1A	3646	1/1	0.95	0.14	46,46,46,46	0
56	MG	2A	3098	1/1	0.95	0.23	55,55,55,55	0
56	MG	1A	3016	1/1	0.95	0.16	39,39,39,39	0
56	MG	2A	3100	1/1	0.95	0.17	56,56,56,56	0
56	MG	1A	3551	1/1	0.95	0.13	59,59,59,59	0
56	MG	1A	4032	1/1	0.95	0.14	21,21,21,21	0
56	MG	1A	3219	1/1	0.95	0.79	37,37,37,37	0
56	MG	1A	3553	1/1	0.95	0.13	25,25,25,25	0
56	MG	1A	4037	1/1	0.95	0.25	55,55,55,55	0
56	MG	1A	3486	1/1	0.95	0.36	54,54,54,54	0
56	MG	1A	3350	1/1	0.95	0.65	50,50,50,50	0
56	MG	27	101	1/1	0.95	0.96	42,42,42,42	0
56	MG	1a	1619	1/1	0.95	0.11	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	3545	1/1	0.95	0.13	44,44,44,44	0
56	MG	1A	3161	1/1	0.95	0.34	47,47,47,47	0
56	MG	1A	3294	1/1	0.95	0.31	62,62,62,62	0
56	MG	2A	3556	1/1	0.95	0.16	51,51,51,51	0
56	MG	1A	3911	1/1	0.95	0.09	26,26,26,26	0
56	MG	2a	3007	1/1	0.95	0.15	55,55,55,55	0
56	MG	2A	3558	1/1	0.95	0.10	36,36,36,36	0
56	MG	1a	1782	1/1	0.95	0.10	49,49,49,49	0
56	MG	1A	3083	1/1	0.95	0.24	39,39,39,39	0
56	MG	1a	1625	1/1	0.95	0.29	44,44,44,44	0
56	MG	1A	3562	1/1	0.95	0.17	43,43,43,43	0
56	MG	2A	3569	1/1	0.95	0.13	41,41,41,41	0
56	MG	2A	3316	1/1	0.95	0.66	53,53,53,53	0
56	MG	2A	3572	1/1	0.95	0.08	57,57,57,57	0
56	MG	1a	1788	1/1	0.95	0.33	60,60,60,60	0
56	MG	2A	3574	1/1	0.95	0.56	61,61,61,61	0
56	MG	2A	3575	1/1	0.95	0.19	37,37,37,37	0
56	MG	2A	3318	1/1	0.95	0.43	53,53,53,53	0
56	MG	2A	3579	1/1	0.95	0.17	67,67,67,67	0
56	MG	1A	3052	1/1	0.95	0.19	41,41,41,41	0
56	MG	2A	3581	1/1	0.95	0.14	54,54,54,54	0
56	MG	1A	3130	1/1	0.95	0.44	41,41,41,41	0
56	MG	1A	3793	1/1	0.95	0.13	45,45,45,45	0
56	MG	2a	3032	1/1	0.95	0.07	37,37,37,37	0
56	MG	2a	3033	1/1	0.95	0.31	57,57,57,57	0
56	MG	1B	211	1/1	0.95	0.18	45,45,45,45	0
56	MG	1A	3669	1/1	0.95	0.11	37,37,37,37	0
56	MG	2A	3133	1/1	0.95	0.20	52,52,52,52	0
56	MG	1A	3441	1/1	0.95	0.62	51,51,51,51	0
56	MG	1A	3231	1/1	0.95	0.12	42,42,42,42	0
56	MG	2A	3137	1/1	0.95	0.18	49,49,49,49	0
56	MG	1A	3798	1/1	0.95	0.18	20,20,20,20	0
56	MG	1a	1800	1/1	0.95	0.09	57,57,57,57	0
56	MG	2A	3333	1/1	0.95	0.09	37,37,37,37	0
56	MG	2A	3603	1/1	0.95	0.17	33,33,33,33	0
56	MG	1a	1801	1/1	0.95	0.07	60,60,60,60	0
56	MG	1a	1803	1/1	0.95	0.14	67,67,67,67	0
56	MG	2A	3336	1/1	0.95	0.47	47,47,47,47	0
56	MG	1A	3268	1/1	0.95	0.78	57,57,57,57	0
56	MG	1A	3569	1/1	0.95	0.13	53,53,53,53	0
56	MG	1A	3571	1/1	0.95	0.20	33,33,33,33	0
56	MG	1A	3805	1/1	0.95	0.10	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	3056	1/1	0.95	0.18	75,75,75,75	0
56	MG	2a	3058	1/1	0.95	0.14	76,76,76,76	0
56	MG	2A	3149	1/1	0.95	0.15	52,52,52,52	0
56	MG	2A	3345	1/1	0.95	0.14	44,44,44,44	0
56	MG	2A	3620	1/1	0.95	0.14	48,48,48,48	0
56	MG	2A	3346	1/1	0.95	0.21	50,50,50,50	0
56	MG	2a	3063	1/1	0.95	0.13	54,54,54,54	0
56	MG	1a	1813	1/1	0.95	0.25	72,72,72,72	0
56	MG	1a	1641	1/1	0.95	0.11	49,49,49,49	0
56	MG	1A	3928	1/1	0.95	0.09	58,58,58,58	0
56	MG	1A	3688	1/1	0.95	0.28	50,50,50,50	0
56	MG	2A	3161	1/1	0.95	0.31	59,59,59,59	0
56	MG	2a	3074	1/1	0.95	0.10	55,55,55,55	0
56	MG	1a	1817	1/1	0.95	0.10	70,70,70,70	0
56	MG	1a	1819	1/1	0.95	0.19	56,56,56,56	0
56	MG	1A	3325	1/1	0.95	0.28	43,43,43,43	0
56	MG	2A	3358	1/1	0.95	0.41	38,38,38,38	0
56	MG	2A	3638	1/1	0.95	0.19	56,56,56,56	0
56	MG	2a	3081	1/1	0.95	0.19	75,75,75,75	0
56	MG	2a	3082	1/1	0.95	0.12	53,53,53,53	0
56	MG	1A	3812	1/1	0.95	0.13	49,49,49,49	0
56	MG	1A	3446	1/1	0.95	0.14	37,37,37,37	0
56	MG	1A	3814	1/1	0.95	0.16	38,38,38,38	0
56	MG	2A	3171	1/1	0.95	0.14	50,50,50,50	0
56	MG	1A	3816	1/1	0.95	0.16	61,61,61,61	0
56	MG	1A	3817	1/1	0.95	0.17	30,30,30,30	0
56	MG	1A	3818	1/1	0.95	0.21	41,41,41,41	0
56	MG	2A	3175	1/1	0.95	0.46	40,40,40,40	0
56	MG	2A	3651	1/1	0.95	0.13	70,70,70,70	0
56	MG	2a	3097	1/1	0.95	0.16	35,35,35,35	0
56	MG	2A	3371	1/1	0.95	0.20	31,31,31,31	0
56	MG	1A	3269	1/1	0.95	0.23	54,54,54,54	0
56	MG	2A	3655	1/1	0.95	0.35	59,59,59,59	0
56	MG	1a	1656	1/1	0.95	0.12	55,55,55,55	0
56	MG	2a	3104	1/1	0.95	0.38	57,57,57,57	0
56	MG	1A	3404	1/1	0.95	0.20	32,32,32,32	0
56	MG	2A	3379	1/1	0.95	0.16	45,45,45,45	0
56	MG	1A	3821	1/1	0.95	0.69	34,34,34,34	0
56	MG	1A	3580	1/1	0.95	0.10	30,30,30,30	0
56	MG	2A	3383	1/1	0.95	0.53	53,53,53,53	0
56	MG	1A	3823	1/1	0.95	0.95	42,42,42,42	0
56	MG	2a	3112	1/1	0.95	0.14	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	3672	1/1	0.95	0.08	46,46,46,46	0
56	MG	1A	3582	1/1	0.95	0.11	39,39,39,39	0
56	MG	1x	102	1/1	0.95	0.15	62,62,62,62	0
56	MG	1x	103	1/1	0.95	0.21	65,65,65,65	0
56	MG	1a	1664	1/1	0.95	0.07	72,72,72,72	0
56	MG	1A	3944	1/1	0.95	0.15	45,45,45,45	0
56	MG	1A	3110	1/1	0.95	0.58	41,41,41,41	0
56	MG	1A	3508	1/1	0.95	0.19	42,42,42,42	0
56	MG	1A	3586	1/1	0.95	0.29	65,65,65,65	0
56	MG	1A	3705	1/1	0.95	0.12	63,63,63,63	0
56	MG	2A	3686	1/1	0.95	0.19	68,68,68,68	0
56	MG	1A	3012	1/1	0.95	0.50	38,38,38,38	0
56	MG	2a	3125	1/1	0.95	0.11	38,38,38,38	0
56	MG	1A	3135	1/1	0.95	0.44	34,34,34,34	0
56	MG	1N	202	1/1	0.95	0.42	46,46,46,46	0
56	MG	2a	3129	1/1	0.95	0.14	62,62,62,62	0
56	MG	1A	3589	1/1	0.95	0.14	37,37,37,37	0
56	MG	2A	3693	1/1	0.95	0.20	48,48,48,48	0
56	MG	2A	3695	1/1	0.95	0.45	51,51,51,51	0
56	MG	2A	3404	1/1	0.95	0.12	51,51,51,51	0
56	MG	2A	3197	1/1	0.95	0.80	45,45,45,45	0
56	MG	1A	3837	1/1	0.95	0.11	41,41,41,41	0
56	MG	2A	3700	1/1	0.95	0.20	61,61,61,61	0
56	MG	2A	3701	1/1	0.95	0.10	51,51,51,51	0
56	MG	1a	1676	1/1	0.95	0.14	35,35,35,35	0
56	MG	1A	3712	1/1	0.95	0.17	42,42,42,42	0
56	MG	1A	3373	1/1	0.95	0.10	33,33,33,33	0
56	MG	2A	3706	1/1	0.95	0.22	65,65,65,65	0
56	MG	2A	3411	1/1	0.95	0.26	52,52,52,52	0
56	MG	2A	3708	1/1	0.95	0.07	45,45,45,45	0
56	MG	1A	3960	1/1	0.95	0.11	27,27,27,27	0
56	MG	2a	3145	1/1	0.95	0.06	67,67,67,67	0
56	MG	1A	3714	1/1	0.95	0.25	26,26,26,26	0
56	MG	2a	3148	1/1	0.95	0.13	60,60,60,60	0
56	MG	1a	1682	1/1	0.95	0.80	57,57,57,57	0
56	MG	2A	3207	1/1	0.95	0.62	46,46,46,46	0
56	MG	1A	3374	1/1	0.95	0.11	38,38,38,38	0
56	MG	1A	3595	1/1	0.95	0.10	41,41,41,41	0
56	MG	2a	3154	1/1	0.95	0.06	69,69,69,69	0
56	MG	1A	3717	1/1	0.95	0.11	32,32,32,32	0
56	MG	2A	3429	1/1	0.95	0.49	67,67,67,67	0
56	MG	1A	3139	1/1	0.95	0.17	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3017	1/1	0.95	0.09	46,46,46,46	0
56	MG	1A	3376	1/1	0.95	0.20	26,26,26,26	0
56	MG	2a	3161	1/1	0.95	0.16	58,58,58,58	0
56	MG	2A	3723	1/1	0.95	0.16	59,59,59,59	0
56	MG	2A	3215	1/1	0.95	0.08	54,54,54,54	0
56	MG	2A	3021	1/1	0.95	0.09	54,54,54,54	0
56	MG	2a	3167	1/1	0.95	0.21	54,54,54,54	0
56	MG	1A	3969	1/1	0.95	0.38	62,62,62,62	0
56	MG	2A	3730	1/1	0.95	0.08	71,71,71,71	0
56	MG	2A	3023	1/1	0.95	0.88	55,55,55,55	0
56	MG	1A	3518	1/1	0.95	0.84	52,52,52,52	0
56	MG	1A	3460	1/1	0.95	0.23	44,44,44,44	0
56	MG	1A	3462	1/1	0.95	0.29	43,43,43,43	0
56	MG	2a	3174	1/1	0.95	0.27	78,78,78,78	0
56	MG	1A	3609	1/1	0.95	0.16	42,42,42,42	0
56	MG	1A	3523	1/1	0.95	0.10	46,46,46,46	0
56	MG	1A	3306	1/1	0.95	0.13	55,55,55,55	0
56	MG	1A	3048	1/1	0.95	0.17	28,28,28,28	0
56	MG	2A	3449	1/1	0.95	0.07	67,67,67,67	0
56	MG	2A	3742	1/1	0.95	0.09	43,43,43,43	0
56	MG	2A	3450	1/1	0.95	0.18	51,51,51,51	0
56	MG	2A	3231	1/1	0.95	0.64	56,56,56,56	0
56	MG	1a	1697	1/1	0.95	0.26	67,67,67,67	0
56	MG	1A	3015	1/1	0.95	0.57	47,47,47,47	0
56	MG	2A	3234	1/1	0.95	0.10	50,50,50,50	0
56	MG	2A	3748	1/1	0.95	0.12	47,47,47,47	0
56	MG	1a	1705	1/1	0.95	0.30	45,45,45,45	0
56	MG	2A	3751	1/1	0.95	0.12	54,54,54,54	0
56	MG	2a	3194	1/1	0.95	0.17	71,71,71,71	0
56	MG	1A	3466	1/1	0.95	0.79	51,51,51,51	0
56	MG	1A	3041	1/1	0.95	0.46	45,45,45,45	0
56	MG	1V	205	1/1	0.95	0.18	49,49,49,49	0
56	MG	2A	3756	1/1	0.95	0.12	34,34,34,34	0
56	MG	2a	3203	1/1	0.95	0.38	64,64,64,64	0
56	MG	2a	3204	1/1	0.95	0.11	58,58,58,58	0
56	MG	2A	3757	1/1	0.95	0.07	59,59,59,59	0
56	MG	1A	3078	1/1	0.95	0.69	47,47,47,47	0
56	MG	2A	3462	1/1	0.95	0.15	54,54,54,54	0
56	MG	2A	3761	1/1	0.95	0.08	55,55,55,55	0
56	MG	2a	3210	1/1	0.95	0.17	58,58,58,58	0
56	MG	2a	3212	1/1	0.95	0.10	67,67,67,67	0
56	MG	2A	3044	1/1	0.95	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	3623	1/1	0.95	0.12	21,21,21,21	0
56	MG	1A	3214	1/1	0.95	0.12	50,50,50,50	0
56	MG	1X	102	1/1	0.95	0.31	49,49,49,49	0
56	MG	2A	3767	1/1	0.95	0.18	62,62,62,62	0
56	MG	1A	3535	1/1	0.95	0.12	28,28,28,28	0
56	MG	1A	3628	1/1	0.95	0.12	40,40,40,40	0
56	MG	2f	201	1/1	0.95	0.20	49,49,49,49	0
56	MG	2A	3469	1/1	0.95	0.11	53,53,53,53	0
56	MG	1A	3992	1/1	0.95	0.16	40,40,40,40	0
56	MG	1A	3244	1/1	0.95	0.27	49,49,49,49	0
56	MG	2n	101	1/1	0.95	0.13	60,60,60,60	0
56	MG	1a	1721	1/1	0.95	0.19	66,66,66,66	0
56	MG	1a	1722	1/1	0.95	0.22	51,51,51,51	0
56	MG	2t	201	1/1	0.95	0.09	53,53,53,53	0
56	MG	1A	3630	1/1	0.95	0.28	65,65,65,65	0
56	MG	1A	3879	1/1	0.95	0.21	36,36,36,36	0
56	MG	1A	3999	1/1	0.95	0.08	45,45,45,45	0
56	MG	2x	103	1/1	0.95	0.16	59,59,59,59	0
56	MG	2A	3060	1/1	0.95	0.27	44,44,44,44	0
56	MG	2A	3790	1/1	0.95	0.14	62,62,62,62	0
56	MG	1A	4004	1/1	0.95	0.09	46,46,46,46	0
56	MG	1A	4006	1/1	0.95	0.23	54,54,54,54	0
56	MG	1A	3080	1/1	0.95	0.46	31,31,31,31	0
56	MG	2A	3795	1/1	0.96	0.10	44,44,44,44	0
56	MG	2A	3796	1/1	0.96	0.08	53,53,53,53	0
56	MG	1O	202	1/1	0.96	0.24	56,56,56,56	0
56	MG	2A	3798	1/1	0.96	0.12	59,59,59,59	0
56	MG	1a	1688	1/1	0.96	0.12	52,52,52,52	0
56	MG	2A	3800	1/1	0.96	0.10	38,38,38,38	0
56	MG	2A	3801	1/1	0.96	0.25	59,59,59,59	0
56	MG	1A	3007	1/1	0.96	0.41	45,45,45,45	0
56	MG	1A	3952	1/1	0.96	0.12	40,40,40,40	0
56	MG	2A	3805	1/1	0.96	0.09	43,43,43,43	0
56	MG	1A	3699	1/1	0.96	0.21	58,58,58,58	0
56	MG	1A	3239	1/1	0.96	0.56	42,42,42,42	0
56	MG	2A	3809	1/1	0.96	0.11	38,38,38,38	0
56	MG	2A	3810	1/1	0.96	0.12	51,51,51,51	0
56	MG	2A	3492	1/1	0.96	0.14	49,49,49,49	0
56	MG	2B	202	1/1	0.96	0.08	56,56,56,56	0
56	MG	2A	3249	1/1	0.96	0.29	55,55,55,55	0
56	MG	1A	3192	1/1	0.96	0.41	44,44,44,44	0
56	MG	1A	3352	1/1	0.96	0.74	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	3496	1/1	0.96	0.12	45,45,45,45	0
56	MG	1R	202	1/1	0.96	0.31	51,51,51,51	0
56	MG	2B	208	1/1	0.96	0.20	48,48,48,48	0
56	MG	2A	3043	1/1	0.96	0.09	58,58,58,58	0
56	MG	1A	3491	1/1	0.96	0.36	44,44,44,44	0
56	MG	1A	3099	1/1	0.96	0.50	33,33,33,33	0
56	MG	1a	1700	1/1	0.96	0.17	48,48,48,48	0
56	MG	1A	3195	1/1	0.96	0.34	45,45,45,45	0
56	MG	2B	215	1/1	0.96	0.35	71,71,71,71	0
56	MG	1a	1704	1/1	0.96	0.14	38,38,38,38	0
56	MG	1A	3708	1/1	0.96	0.14	46,46,46,46	0
56	MG	1A	3138	1/1	0.96	0.73	37,37,37,37	0
56	MG	1A	3102	1/1	0.96	0.83	38,38,38,38	0
56	MG	2A	3264	1/1	0.96	0.08	38,38,38,38	0
56	MG	1a	1709	1/1	0.96	0.20	56,56,56,56	0
56	MG	1A	3838	1/1	0.96	0.14	41,41,41,41	0
56	MG	2A	3055	1/1	0.96	0.09	59,59,59,59	0
56	MG	1U	201	1/1	0.96	0.99	42,42,42,42	0
56	MG	2E	308	1/1	0.96	0.38	51,51,51,51	0
56	MG	2E	309	1/1	0.96	0.23	39,39,39,39	0
56	MG	1A	3103	1/1	0.96	0.60	42,42,42,42	0
56	MG	2A	3270	1/1	0.96	0.11	56,56,56,56	0
56	MG	2A	3517	1/1	0.96	0.31	73,73,73,73	0
56	MG	1A	3498	1/1	0.96	0.07	38,38,38,38	0
56	MG	2A	3272	1/1	0.96	0.21	46,46,46,46	0
56	MG	2A	3274	1/1	0.96	0.31	48,48,48,48	0
56	MG	2A	3059	1/1	0.96	0.12	52,52,52,52	0
56	MG	2R	204	1/1	0.96	0.24	42,42,42,42	0
56	MG	1A	3841	1/1	0.96	0.20	48,48,48,48	0
56	MG	1A	3248	1/1	0.96	0.42	53,53,53,53	0
56	MG	2T	203	1/1	0.96	0.48	34,34,34,34	0
56	MG	2A	3062	1/1	0.96	0.72	71,71,71,71	0
56	MG	2U	202	1/1	0.96	0.14	44,44,44,44	0
56	MG	1A	3420	1/1	0.96	0.58	37,37,37,37	0
56	MG	2A	3530	1/1	0.96	0.21	46,46,46,46	0
56	MG	1A	3847	1/1	0.96	0.13	30,30,30,30	0
56	MG	1A	3146	1/1	0.96	0.62	42,42,42,42	0
56	MG	1V	201	1/1	0.96	0.93	39,39,39,39	0
56	MG	1V	203	1/1	0.96	0.57	44,44,44,44	0
56	MG	1a	1723	1/1	0.96	0.35	50,50,50,50	0
56	MG	1A	3975	1/1	0.96	0.17	63,63,63,63	0
56	MG	1a	1726	1/1	0.96	0.17	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	3594	1/1	0.96	0.24	36,36,36,36	0
56	MG	1A	3019	1/1	0.96	0.08	48,48,48,48	0
56	MG	2A	3075	1/1	0.96	0.15	52,52,52,52	0
56	MG	1W	201	1/1	0.96	0.26	33,33,33,33	0
56	MG	2A	3553	1/1	0.96	0.10	43,43,43,43	0
56	MG	2A	3077	1/1	0.96	0.17	42,42,42,42	0
56	MG	1A	3154	1/1	0.96	0.22	37,37,37,37	0
56	MG	2a	3004	1/1	0.96	0.27	47,47,47,47	0
56	MG	1A	3155	1/1	0.96	0.47	41,41,41,41	0
56	MG	1A	3598	1/1	0.96	0.21	57,57,57,57	0
56	MG	1A	3368	1/1	0.96	0.66	32,32,32,32	0
56	MG	1X	105	1/1	0.96	0.12	45,45,45,45	0
56	MG	2A	3561	1/1	0.96	0.27	59,59,59,59	0
56	MG	1A	3369	1/1	0.96	0.88	41,41,41,41	0
56	MG	2A	3563	1/1	0.96	0.14	36,36,36,36	0
56	MG	1A	3077	1/1	0.96	0.20	38,38,38,38	0
56	MG	1a	1740	1/1	0.96	0.17	37,37,37,37	0
56	MG	1A	3512	1/1	0.96	0.23	42,42,42,42	0
56	MG	1a	1742	1/1	0.96	0.11	52,52,52,52	0
56	MG	2A	3089	1/1	0.96	0.23	61,61,61,61	0
56	MG	1A	3371	1/1	0.96	1.26	59,59,59,59	0
56	MG	2A	3091	1/1	0.96	0.34	54,54,54,54	0
56	MG	2A	3577	1/1	0.96	0.10	70,70,70,70	0
56	MG	2A	3092	1/1	0.96	0.09	53,53,53,53	0
56	MG	2a	3024	1/1	0.96	0.80	53,53,53,53	0
56	MG	1a	1745	1/1	0.96	0.13	49,49,49,49	0
56	MG	2a	3026	1/1	0.96	0.79	48,48,48,48	0
56	MG	1A	3732	1/1	0.96	0.17	49,49,49,49	0
56	MG	1A	3991	1/1	0.96	0.12	31,31,31,31	0
56	MG	10	104	1/1	0.96	0.10	46,46,46,46	0
56	MG	2a	3031	1/1	0.96	0.07	81,81,81,81	0
56	MG	1A	3734	1/1	0.96	0.17	40,40,40,40	0
56	MG	1A	3008	1/1	0.96	0.11	34,34,34,34	0
56	MG	1A	3994	1/1	0.96	0.10	39,39,39,39	0
56	MG	1A	3736	1/1	0.96	0.16	25,25,25,25	0
56	MG	11	101	1/1	0.96	0.14	39,39,39,39	0
56	MG	1A	3062	1/1	0.96	0.10	49,49,49,49	0
56	MG	1A	3998	1/1	0.96	0.10	37,37,37,37	0
56	MG	2A	3107	1/1	0.96	0.28	39,39,39,39	0
56	MG	2A	3598	1/1	0.96	0.30	60,60,60,60	0
56	MG	1A	3258	1/1	0.96	0.09	53,53,53,53	0
56	MG	1A	4001	1/1	0.96	0.14	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3602	1/1	0.96	0.07	64,64,64,64	0
56	MG	15	104	1/1	0.96	0.96	38,38,38,38	0
56	MG	2A	3604	1/1	0.96	0.20	38,38,38,38	0
56	MG	1A	3260	1/1	0.96	0.30	36,36,36,36	0
56	MG	2A	3330	1/1	0.96	0.11	71,71,71,71	0
56	MG	2a	3049	1/1	0.96	0.36	44,44,44,44	0
56	MG	16	101	1/1	0.96	0.48	44,44,44,44	0
56	MG	2a	3053	1/1	0.96	0.31	54,54,54,54	0
56	MG	2A	3610	1/1	0.96	0.11	48,48,48,48	0
56	MG	2A	3611	1/1	0.96	0.10	31,31,31,31	0
56	MG	1a	1764	1/1	0.96	0.23	60,60,60,60	0
56	MG	2A	3613	1/1	0.96	0.14	55,55,55,55	0
56	MG	1A	3377	1/1	0.96	0.40	33,33,33,33	0
56	MG	1A	3378	1/1	0.96	0.17	50,50,50,50	0
56	MG	2A	3116	1/1	0.96	0.46	68,68,68,68	0
56	MG	17	104	1/1	0.96	0.18	36,36,36,36	0
56	MG	2A	3618	1/1	0.96	0.28	59,59,59,59	0
56	MG	2a	3065	1/1	0.96	0.29	47,47,47,47	0
56	MG	2A	3337	1/1	0.96	0.16	56,56,56,56	0
56	MG	1A	3521	1/1	0.96	0.49	38,38,38,38	0
56	MG	1A	3443	1/1	0.96	0.77	44,44,44,44	0
56	MG	2a	3070	1/1	0.96	0.42	44,44,44,44	0
56	MG	1A	4011	1/1	0.96	0.09	52,52,52,52	0
56	MG	2A	3624	1/1	0.96	0.11	49,49,49,49	0
56	MG	2a	3073	1/1	0.96	0.17	66,66,66,66	0
56	MG	2A	3625	1/1	0.96	0.09	58,58,58,58	0
56	MG	1A	3625	1/1	0.96	0.12	34,34,34,34	0
56	MG	18	102	1/1	0.96	0.22	42,42,42,42	0
56	MG	2A	3125	1/1	0.96	0.46	46,46,46,46	0
56	MG	2A	3629	1/1	0.96	0.20	56,56,56,56	0
56	MG	1a	1776	1/1	0.96	0.08	56,56,56,56	0
56	MG	1A	3042	1/1	0.96	0.19	33,33,33,33	0
56	MG	1A	3263	1/1	0.96	0.35	36,36,36,36	0
56	MG	1A	3210	1/1	0.96	0.15	52,52,52,52	0
56	MG	2a	3085	1/1	0.96	0.12	67,67,67,67	0
56	MG	1a	1780	1/1	0.96	0.12	74,74,74,74	0
56	MG	2a	3087	1/1	0.96	0.07	76,76,76,76	0
56	MG	1A	3043	1/1	0.96	0.15	36,36,36,36	0
56	MG	1A	4019	1/1	0.96	0.12	53,53,53,53	0
56	MG	2A	3354	1/1	0.96	0.25	51,51,51,51	0
56	MG	1A	3084	1/1	0.96	0.32	50,50,50,50	0
56	MG	1a	1605	1/1	0.96	0.10	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	3643	1/1	0.96	0.12	61,61,61,61	0
56	MG	2A	3644	1/1	0.96	0.23	58,58,58,58	0
56	MG	1A	3755	1/1	0.96	0.10	58,58,58,58	0
56	MG	2A	3141	1/1	0.96	0.14	64,64,64,64	0
56	MG	1A	3633	1/1	0.96	0.21	23,23,23,23	0
56	MG	1A	3531	1/1	0.96	1.01	53,53,53,53	0
56	MG	1A	4024	1/1	0.96	0.40	61,61,61,61	0
56	MG	2A	3145	1/1	0.96	0.12	49,49,49,49	0
56	MG	1a	1610	1/1	0.96	0.81	66,66,66,66	0
56	MG	2A	3654	1/1	0.96	0.06	62,62,62,62	0
56	MG	2A	3365	1/1	0.96	0.13	46,46,46,46	0
56	MG	2A	3656	1/1	0.96	0.27	66,66,66,66	0
56	MG	1a	1792	1/1	0.96	0.28	53,53,53,53	0
56	MG	2A	3148	1/1	0.96	0.12	50,50,50,50	0
56	MG	2A	3370	1/1	0.96	0.17	62,62,62,62	0
56	MG	2A	3661	1/1	0.96	0.20	62,62,62,62	0
56	MG	1a	1611	1/1	0.96	0.19	28,28,28,28	0
56	MG	2A	3663	1/1	0.96	0.13	50,50,50,50	0
56	MG	1a	1612	1/1	0.96	0.14	35,35,35,35	0
56	MG	2A	3373	1/1	0.96	0.18	41,41,41,41	0
56	MG	2A	3669	1/1	0.96	0.33	43,43,43,43	0
56	MG	2A	3670	1/1	0.96	0.16	62,62,62,62	0
56	MG	2A	3375	1/1	0.96	0.19	37,37,37,37	0
56	MG	2A	3152	1/1	0.96	0.10	47,47,47,47	0
56	MG	2A	3155	1/1	0.96	0.17	41,41,41,41	0
56	MG	1A	3032	1/1	0.96	0.77	47,47,47,47	0
56	MG	1a	1615	1/1	0.96	0.14	48,48,48,48	0
56	MG	1A	3452	1/1	0.96	1.06	41,41,41,41	0
56	MG	2A	3160	1/1	0.96	0.26	50,50,50,50	0
56	MG	1A	3534	1/1	0.96	0.12	26,26,26,26	0
56	MG	1A	3894	1/1	0.96	0.08	56,56,56,56	0
56	MG	1A	3046	1/1	0.96	0.12	50,50,50,50	0
56	MG	1a	1804	1/1	0.96	0.15	46,46,46,46	0
56	MG	2A	3389	1/1	0.96	0.25	42,42,42,42	0
56	MG	2A	3687	1/1	0.96	0.14	55,55,55,55	0
56	MG	1A	3896	1/1	0.96	0.09	89,89,89,89	0
56	MG	1A	3764	1/1	0.96	0.46	41,41,41,41	0
56	MG	1A	3767	1/1	0.96	0.22	49,49,49,49	0
56	MG	1A	3170	1/1	0.96	0.31	44,44,44,44	0
56	MG	1a	1811	1/1	0.96	0.06	45,45,45,45	0
56	MG	2A	3694	1/1	0.96	0.14	46,46,46,46	0
56	MG	1A	3537	1/1	0.96	0.26	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	3696	1/1	0.96	0.12	47,47,47,47	0
56	MG	1A	4038	1/1	0.96	0.29	41,41,41,41	0
56	MG	1A	3171	1/1	0.96	0.15	67,67,67,67	0
56	MG	1A	3218	1/1	0.96	0.40	47,47,47,47	0
56	MG	1A	3645	1/1	0.96	0.14	23,23,23,23	0
56	MG	2a	3146	1/1	0.96	0.12	81,81,81,81	0
56	MG	2A	3403	1/1	0.96	0.15	57,57,57,57	0
56	MG	1A	3327	1/1	0.96	1.05	49,49,49,49	0
56	MG	1a	1820	1/1	0.96	0.20	44,44,44,44	0
56	MG	1A	3776	1/1	0.96	0.15	46,46,46,46	0
56	MG	2a	3151	1/1	0.96	0.12	82,82,82,82	0
56	MG	1A	3278	1/1	0.96	0.37	31,31,31,31	0
56	MG	2A	3182	1/1	0.96	0.13	41,41,41,41	0
56	MG	2A	3409	1/1	0.96	0.15	56,56,56,56	0
56	MG	1A	3908	1/1	0.96	0.27	72,72,72,72	0
56	MG	1A	3648	1/1	0.96	0.25	64,64,64,64	0
56	MG	1A	3088	1/1	0.96	0.12	55,55,55,55	0
56	MG	2A	3414	1/1	0.96	0.15	73,73,73,73	0
56	MG	1A	3393	1/1	0.96	0.15	41,41,41,41	0
56	MG	2a	3160	1/1	0.96	0.10	67,67,67,67	0
56	MG	1A	3653	1/1	0.96	0.17	28,28,28,28	0
56	MG	2a	3162	1/1	0.96	0.09	53,53,53,53	0
56	MG	1B	212	1/1	0.96	0.28	41,41,41,41	0
56	MG	2A	3419	1/1	0.96	1.24	60,60,60,60	0
56	MG	1B	213	1/1	0.96	0.11	37,37,37,37	0
56	MG	1A	3915	1/1	0.96	0.11	51,51,51,51	0
56	MG	2A	3423	1/1	0.96	0.28	70,70,70,70	0
56	MG	2A	3424	1/1	0.96	0.16	39,39,39,39	0
56	MG	2A	3724	1/1	0.96	0.10	46,46,46,46	0
56	MG	2A	3426	1/1	0.96	0.20	40,40,40,40	0
56	MG	2A	3727	1/1	0.96	0.14	63,63,63,63	0
56	MG	1A	3220	1/1	0.96	0.09	42,42,42,42	0
56	MG	2A	3428	1/1	0.96	0.13	57,57,57,57	0
56	MG	1A	3123	1/1	0.96	0.86	40,40,40,40	0
56	MG	1A	3222	1/1	0.96	0.15	41,41,41,41	0
56	MG	1B	222	1/1	0.96	0.16	67,67,67,67	0
56	MG	1a	1651	1/1	0.96	0.11	39,39,39,39	0
56	MG	2a	3179	1/1	0.96	0.43	70,70,70,70	0
56	MG	2a	3180	1/1	0.96	0.29	62,62,62,62	0
56	MG	1A	3124	1/1	0.96	0.66	60,60,60,60	0
56	MG	2a	3182	1/1	0.96	0.09	60,60,60,60	0
56	MG	1A	3467	1/1	0.96	0.68	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3227	1/1	0.96	0.20	37,37,37,37	0
56	MG	1x	106	1/1	0.96	0.11	72,72,72,72	0
56	MG	1A	3177	1/1	0.96	0.68	36,36,36,36	0
56	MG	1A	3089	1/1	0.96	0.16	39,39,39,39	0
56	MG	1A	3180	1/1	0.96	0.56	40,40,40,40	0
56	MG	2A	3443	1/1	0.96	0.73	38,38,38,38	0
56	MG	2A	3204	1/1	0.96	0.13	40,40,40,40	0
56	MG	1B	230	1/1	0.96	0.08	61,61,61,61	0
56	MG	1A	3796	1/1	0.96	0.18	51,51,51,51	0
56	MG	1D	303	1/1	0.96	0.81	39,39,39,39	0
56	MG	1A	3667	1/1	0.96	0.20	36,36,36,36	0
56	MG	1A	3402	1/1	0.96	0.35	47,47,47,47	0
56	MG	1A	3800	1/1	0.96	0.20	57,57,57,57	0
56	MG	1A	3035	1/1	0.96	0.15	42,42,42,42	0
56	MG	2A	3004	1/1	0.96	0.15	51,51,51,51	0
56	MG	1A	3014	1/1	0.96	0.09	28,28,28,28	0
56	MG	2A	3006	1/1	0.96	0.18	53,53,53,53	0
56	MG	2a	3207	1/1	0.96	0.30	68,68,68,68	0
56	MG	1A	3674	1/1	0.96	0.08	64,64,64,64	0
56	MG	1A	3477	1/1	0.96	0.20	50,50,50,50	0
56	MG	1A	3676	1/1	0.96	0.15	42,42,42,42	0
56	MG	2A	3459	1/1	0.96	0.18	59,59,59,59	0
56	MG	2A	3223	1/1	0.96	0.33	52,52,52,52	0
56	MG	1A	3807	1/1	0.96	0.61	37,37,37,37	0
56	MG	1E	309	1/1	0.96	0.30	56,56,56,56	0
56	MG	1A	3809	1/1	0.96	0.23	48,48,48,48	0
56	MG	1A	3681	1/1	0.96	0.07	59,59,59,59	0
56	MG	2A	3768	1/1	0.96	0.26	43,43,43,43	0
56	MG	1A	3187	1/1	0.96	0.16	49,49,49,49	0
56	MG	1a	1677	1/1	0.96	0.42	66,66,66,66	0
56	MG	1A	3683	1/1	0.96	0.07	54,54,54,54	0
56	MG	2A	3774	1/1	0.96	0.79	73,73,73,73	0
56	MG	2A	3019	1/1	0.96	0.16	46,46,46,46	0
56	MG	1A	3481	1/1	0.96	1.39	36,36,36,36	0
56	MG	2A	3777	1/1	0.96	0.16	65,65,65,65	0
56	MG	1A	3686	1/1	0.96	0.14	47,47,47,47	0
56	MG	1A	3482	1/1	0.96	1.21	37,37,37,37	0
56	MG	1A	3070	1/1	0.96	0.29	43,43,43,43	0
56	MG	2A	3785	1/1	0.96	0.12	41,41,41,41	0
56	MG	1A	3570	1/1	0.96	0.15	40,40,40,40	0
56	MG	1A	3074	1/1	0.96	0.42	42,42,42,42	0
56	MG	2A	3480	1/1	0.96	0.10	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	2x	105	1/1	0.96	0.14	59,59,59,59	0
56	MG	2A	3481	1/1	0.96	0.20	54,54,54,54	0
56	MG	1A	3949	1/1	0.96	0.09	55,55,55,55	0
57	ZN	29	501	1/1	0.96	0.13	72,72,72,72	0
56	MG	2A	3792	1/1	0.96	0.32	63,63,63,63	0
56	MG	1A	3572	1/1	0.96	0.12	34,34,34,34	0
56	MG	1A	3100	1/1	0.97	0.44	37,37,37,37	0
56	MG	1A	3641	1/1	0.97	0.18	56,56,56,56	0
56	MG	1B	218	1/1	0.97	0.14	36,36,36,36	0
56	MG	1A	3461	1/1	0.97	0.12	54,54,54,54	0
56	MG	1B	220	1/1	0.97	0.21	56,56,56,56	0
56	MG	1A	3731	1/1	0.97	0.29	56,56,56,56	0
56	MG	2a	3010	1/1	0.97	0.10	70,70,70,70	0
56	MG	1A	3185	1/1	0.97	0.11	32,32,32,32	0
56	MG	2a	3012	1/1	0.97	0.09	47,47,47,47	0
56	MG	1a	1755	1/1	0.97	0.09	55,55,55,55	0
56	MG	1A	3733	1/1	0.97	0.16	66,66,66,66	0
56	MG	1a	1614	1/1	0.97	0.08	72,72,72,72	0
56	MG	1A	3940	1/1	0.97	0.19	79,79,79,79	0
56	MG	1a	1616	1/1	0.97	0.07	64,64,64,64	0
56	MG	2A	3433	1/1	0.97	0.15	29,29,29,29	0
56	MG	1A	3152	1/1	0.97	0.40	42,42,42,42	0
56	MG	2A	3245	1/1	0.97	0.30	49,49,49,49	0
56	MG	1A	3329	1/1	0.97	0.58	44,44,44,44	0
56	MG	1A	3188	1/1	0.97	0.08	48,48,48,48	0
56	MG	1A	3577	1/1	0.97	0.16	52,52,52,52	0
56	MG	1A	3153	1/1	0.97	0.21	36,36,36,36	0
56	MG	1B	231	1/1	0.97	0.20	36,36,36,36	0
56	MG	2A	3664	1/1	0.97	0.10	43,43,43,43	0
56	MG	2A	3441	1/1	0.97	0.06	47,47,47,47	0
56	MG	2A	3667	1/1	0.97	0.14	37,37,37,37	0
56	MG	2a	3030	1/1	0.97	0.23	64,64,64,64	0
56	MG	1A	3650	1/1	0.97	0.15	26,26,26,26	0
56	MG	1A	3651	1/1	0.97	0.26	30,30,30,30	0
56	MG	1A	3121	1/1	0.97	0.14	61,61,61,61	0
56	MG	1A	3843	1/1	0.97	0.26	52,52,52,52	0
56	MG	1A	3055	1/1	0.97	0.17	41,41,41,41	0
56	MG	2A	3257	1/1	0.97	0.46	47,47,47,47	0
56	MG	1a	1629	1/1	0.97	0.19	46,46,46,46	0
56	MG	1A	3846	1/1	0.97	0.10	53,53,53,53	0
56	MG	1A	3581	1/1	0.97	0.14	31,31,31,31	0
56	MG	1E	304	1/1	0.97	0.24	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	3041	1/1	0.97	0.09	55,55,55,55	0
56	MG	1A	3657	1/1	0.97	0.10	48,48,48,48	0
56	MG	1A	3028	1/1	0.97	0.41	34,34,34,34	0
56	MG	1A	3583	1/1	0.97	0.17	64,64,64,64	0
56	MG	1A	3958	1/1	0.97	0.07	38,38,38,38	0
56	MG	1a	1783	1/1	0.97	0.06	59,59,59,59	0
56	MG	1A	3036	1/1	0.97	0.19	27,27,27,27	0
56	MG	1A	3853	1/1	0.97	0.18	47,47,47,47	0
56	MG	2A	3689	1/1	0.97	0.22	46,46,46,46	0
56	MG	1F	302	1/1	0.97	0.29	53,53,53,53	0
56	MG	2a	3051	1/1	0.97	0.43	81,81,81,81	0
56	MG	2A	3461	1/1	0.97	0.13	47,47,47,47	0
56	MG	1A	3336	1/1	0.97	0.17	56,56,56,56	0
56	MG	1A	3752	1/1	0.97	0.08	42,42,42,42	0
56	MG	1A	3753	1/1	0.97	0.10	31,31,31,31	0
56	MG	1A	3472	1/1	0.97	0.14	49,49,49,49	0
56	MG	1A	3259	1/1	0.97	0.19	37,37,37,37	0
56	MG	1A	3125	1/1	0.97	0.19	42,42,42,42	0
56	MG	1a	1647	1/1	0.97	0.14	48,48,48,48	0
56	MG	2A	3103	1/1	0.97	0.10	32,32,32,32	0
56	MG	1A	3261	1/1	0.97	0.63	62,62,62,62	0
56	MG	1a	1649	1/1	0.97	0.34	62,62,62,62	0
56	MG	1a	1650	1/1	0.97	0.15	55,55,55,55	0
56	MG	2A	3703	1/1	0.97	0.20	38,38,38,38	0
56	MG	1a	1799	1/1	0.97	0.09	66,66,66,66	0
56	MG	2a	3069	1/1	0.97	0.19	53,53,53,53	0
56	MG	1A	3385	1/1	0.97	0.36	48,48,48,48	0
56	MG	1A	3478	1/1	0.97	0.07	48,48,48,48	0
56	MG	2A	3479	1/1	0.97	0.87	40,40,40,40	0
56	MG	1a	1802	1/1	0.97	0.10	64,64,64,64	0
56	MG	1N	201	1/1	0.97	0.64	52,52,52,52	0
56	MG	1A	3761	1/1	0.97	0.14	60,60,60,60	0
56	MG	1a	1805	1/1	0.97	0.18	44,44,44,44	0
56	MG	1a	1806	1/1	0.97	0.07	65,65,65,65	0
56	MG	1A	3670	1/1	0.97	0.12	25,25,25,25	0
56	MG	1A	3869	1/1	0.97	0.06	43,43,43,43	0
56	MG	2A	3487	1/1	0.97	0.14	30,30,30,30	0
56	MG	1P	202	1/1	0.97	0.70	33,33,33,33	0
56	MG	1P	203	1/1	0.97	0.47	43,43,43,43	0
56	MG	2a	3084	1/1	0.97	0.26	52,52,52,52	0
56	MG	1A	3196	1/1	0.97	0.42	37,37,37,37	0
56	MG	1a	1812	1/1	0.97	0.11	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3429	1/1	0.97	0.71	54,54,54,54	0
56	MG	1A	3765	1/1	0.97	0.08	53,53,53,53	0
56	MG	1A	3766	1/1	0.97	0.12	48,48,48,48	0
56	MG	1A	3980	1/1	0.97	0.08	40,40,40,40	0
56	MG	1A	3981	1/1	0.97	0.11	40,40,40,40	0
56	MG	2A	3132	1/1	0.97	0.20	40,40,40,40	0
56	MG	2a	3094	1/1	0.97	0.07	49,49,49,49	0
56	MG	1a	1818	1/1	0.97	0.12	44,44,44,44	0
56	MG	2A	3500	1/1	0.97	0.09	54,54,54,54	0
56	MG	1A	3106	1/1	0.97	1.15	49,49,49,49	0
56	MG	2A	3135	1/1	0.97	0.23	36,36,36,36	0
56	MG	1A	3983	1/1	0.97	0.10	47,47,47,47	0
56	MG	1A	3264	1/1	0.97	0.79	45,45,45,45	0
56	MG	2A	3505	1/1	0.97	0.11	34,34,34,34	0
56	MG	1A	3877	1/1	0.97	0.08	52,52,52,52	0
56	MG	2A	3739	1/1	0.97	0.25	62,62,62,62	0
56	MG	1e	201	1/1	0.97	0.15	42,42,42,42	0
56	MG	1A	3037	1/1	0.97	0.42	37,37,37,37	0
56	MG	1A	3677	1/1	0.97	0.06	31,31,31,31	0
56	MG	1A	3771	1/1	0.97	0.21	40,40,40,40	0
56	MG	1A	3883	1/1	0.97	0.12	34,34,34,34	0
56	MG	1A	3679	1/1	0.97	0.12	31,31,31,31	0
56	MG	1A	3108	1/1	0.97	0.10	43,43,43,43	0
56	MG	1A	3044	1/1	0.97	0.12	40,40,40,40	0
56	MG	1A	3604	1/1	0.97	0.14	25,25,25,25	0
56	MG	1A	3271	1/1	0.97	0.14	27,27,27,27	0
56	MG	1A	3541	1/1	0.97	0.18	51,51,51,51	0
56	MG	2A	3752	1/1	0.97	0.17	44,44,44,44	0
56	MG	2A	3150	1/1	0.97	0.36	54,54,54,54	0
56	MG	2A	3326	1/1	0.97	0.14	66,66,66,66	0
56	MG	1A	3489	1/1	0.97	0.09	58,58,58,58	0
56	MG	2A	3328	1/1	0.97	0.55	65,65,65,65	0
56	MG	1A	3782	1/1	0.97	0.06	38,38,38,38	0
56	MG	2A	3154	1/1	0.97	0.10	68,68,68,68	0
56	MG	1A	3689	1/1	0.97	0.10	45,45,45,45	0
56	MG	1A	4002	1/1	0.97	0.07	47,47,47,47	0
56	MG	2A	3762	1/1	0.97	0.10	65,65,65,65	0
56	MG	2a	3128	1/1	0.97	0.05	67,67,67,67	0
56	MG	1A	3611	1/1	0.97	0.17	29,29,29,29	0
56	MG	1A	3613	1/1	0.97	0.12	43,43,43,43	0
56	MG	2A	3159	1/1	0.97	0.10	45,45,45,45	0
56	MG	1A	3786	1/1	0.97	0.09	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3614	1/1	0.97	0.17	36,36,36,36	0
56	MG	1A	3897	1/1	0.97	0.16	60,60,60,60	0
56	MG	2A	3769	1/1	0.97	0.12	61,61,61,61	0
56	MG	2A	3539	1/1	0.97	0.13	38,38,38,38	0
56	MG	2A	3540	1/1	0.97	0.20	53,53,53,53	0
56	MG	2A	3339	1/1	0.97	0.20	47,47,47,47	0
56	MG	1W	204	1/1	0.97	0.86	36,36,36,36	0
56	MG	2A	3543	1/1	0.97	0.07	35,35,35,35	0
56	MG	2A	3164	1/1	0.97	0.26	57,57,57,57	0
56	MG	1W	205	1/1	0.97	0.39	39,39,39,39	0
56	MG	2A	3547	1/1	0.97	0.10	44,44,44,44	0
56	MG	2A	3550	1/1	0.97	0.10	62,62,62,62	0
56	MG	2A	3781	1/1	0.97	0.35	52,52,52,52	0
56	MG	2A	3782	1/1	0.97	0.24	56,56,56,56	0
56	MG	2A	3166	1/1	0.97	0.10	48,48,48,48	0
56	MG	1x	111	1/1	0.97	0.10	70,70,70,70	0
56	MG	2A	3554	1/1	0.97	0.46	58,58,58,58	0
56	MG	1A	3093	1/1	0.97	0.15	50,50,50,50	0
56	MG	1x	113	1/1	0.97	0.23	63,63,63,63	0
56	MG	1A	3235	1/1	0.97	0.11	50,50,50,50	0
56	MG	1A	3697	1/1	0.97	0.22	42,42,42,42	0
56	MG	1A	3698	1/1	0.97	0.10	35,35,35,35	0
56	MG	1A	3792	1/1	0.97	0.28	51,51,51,51	0
56	MG	1a	1698	1/1	0.97	0.09	43,43,43,43	0
56	MG	1a	1699	1/1	0.97	0.25	41,41,41,41	0
56	MG	1A	4016	1/1	0.97	0.20	40,40,40,40	0
56	MG	2A	3356	1/1	0.97	0.18	55,55,55,55	0
56	MG	2A	3568	1/1	0.97	0.24	40,40,40,40	0
56	MG	1A	3617	1/1	0.97	0.10	27,27,27,27	0
56	MG	1a	1702	1/1	0.97	0.13	51,51,51,51	0
56	MG	2a	3163	1/1	0.97	0.23	50,50,50,50	0
56	MG	2A	3008	1/1	0.97	0.12	58,58,58,58	0
56	MG	1a	1703	1/1	0.97	0.30	58,58,58,58	0
56	MG	1A	3618	1/1	0.97	0.18	27,27,27,27	0
56	MG	1A	3004	1/1	0.97	0.29	38,38,38,38	0
56	MG	2A	3576	1/1	0.97	0.45	47,47,47,47	0
56	MG	1a	1706	1/1	0.97	0.13	62,62,62,62	0
56	MG	1A	3114	1/1	0.97	0.42	43,43,43,43	0
56	MG	1A	3550	1/1	0.97	0.13	27,27,27,27	0
56	MG	1A	3172	1/1	0.97	0.11	48,48,48,48	0
56	MG	2A	3367	1/1	0.97	0.11	41,41,41,41	0
56	MG	1a	1711	1/1	0.97	0.10	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3356	1/1	0.97	0.60	51,51,51,51	0
56	MG	2A	3584	1/1	0.97	0.09	48,48,48,48	0
56	MG	1A	3910	1/1	0.97	0.13	19,19,19,19	0
56	MG	2A	3020	1/1	0.97	0.70	55,55,55,55	0
56	MG	1A	3707	1/1	0.97	0.21	41,41,41,41	0
56	MG	2B	210	1/1	0.97	0.25	42,42,42,42	0
56	MG	2A	3590	1/1	0.97	0.13	37,37,37,37	0
56	MG	1A	3136	1/1	0.97	0.14	35,35,35,35	0
56	MG	1A	3709	1/1	0.97	0.14	28,28,28,28	0
56	MG	1A	3914	1/1	0.97	0.27	54,54,54,54	0
56	MG	1A	3137	1/1	0.97	0.22	39,39,39,39	0
56	MG	15	101	1/1	0.97	0.75	36,36,36,36	0
56	MG	2D	302	1/1	0.97	0.36	62,62,62,62	0
56	MG	2A	3381	1/1	0.97	0.15	33,33,33,33	0
56	MG	1A	3280	1/1	0.97	0.36	35,35,35,35	0
56	MG	1A	4033	1/1	0.97	0.10	34,34,34,34	0
56	MG	2A	3384	1/1	0.97	0.31	37,37,37,37	0
56	MG	1A	3281	1/1	0.97	0.30	44,44,44,44	0
56	MG	2A	3032	1/1	0.97	0.10	47,47,47,47	0
56	MG	1A	3284	1/1	0.97	0.14	38,38,38,38	0
56	MG	2a	3197	1/1	0.97	0.18	58,58,58,58	0
56	MG	2E	306	1/1	0.97	0.56	53,53,53,53	0
56	MG	2a	3199	1/1	0.97	0.22	59,59,59,59	0
56	MG	1A	3560	1/1	0.97	0.21	47,47,47,47	0
56	MG	2a	3201	1/1	0.97	0.12	49,49,49,49	0
56	MG	2a	3202	1/1	0.97	0.15	53,53,53,53	0
56	MG	2A	3609	1/1	0.97	0.14	45,45,45,45	0
56	MG	17	101	1/1	0.97	0.51	39,39,39,39	0
56	MG	1A	3631	1/1	0.97	0.17	35,35,35,35	0
56	MG	2F	302	1/1	0.97	0.14	54,54,54,54	0
56	MG	17	103	1/1	0.97	0.95	48,48,48,48	0
56	MG	2O	201	1/1	0.97	0.07	61,61,61,61	0
56	MG	1a	1729	1/1	0.97	0.13	44,44,44,44	0
56	MG	1A	3503	1/1	0.97	0.19	25,25,25,25	0
56	MG	1A	3010	1/1	0.97	0.22	44,44,44,44	0
56	MG	1A	3815	1/1	0.97	0.64	58,58,58,58	0
56	MG	1A	3924	1/1	0.97	0.20	67,67,67,67	0
56	MG	2A	3398	1/1	0.97	0.14	33,33,33,33	0
56	MG	2A	3399	1/1	0.97	0.17	41,41,41,41	0
56	MG	2A	3214	1/1	0.97	0.11	48,48,48,48	0
56	MG	1A	3563	1/1	0.97	0.20	45,45,45,45	0
56	MG	2A	3622	1/1	0.97	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	3216	1/1	0.97	0.29	37,37,37,37	0
56	MG	2A	3217	1/1	0.97	0.65	46,46,46,46	0
56	MG	1A	3072	1/1	0.97	0.22	45,45,45,45	0
56	MG	1A	3720	1/1	0.97	0.10	21,21,21,21	0
56	MG	1A	3140	1/1	0.97	0.07	48,48,48,48	0
56	MG	2A	3221	1/1	0.97	0.40	58,58,58,58	0
56	MG	1a	1739	1/1	0.97	0.17	38,38,38,38	0
56	MG	2A	3631	1/1	0.97	0.14	68,68,68,68	0
56	MG	1A	3507	1/1	0.97	0.22	40,40,40,40	0
56	MG	2A	3633	1/1	0.97	0.12	51,51,51,51	0
56	MG	2A	3051	1/1	0.97	0.11	56,56,56,56	0
56	MG	25	102	1/1	0.97	0.61	52,52,52,52	0
56	MG	25	103	1/1	0.97	0.44	46,46,46,46	0
56	MG	1A	3723	1/1	0.97	0.08	37,37,37,37	0
56	MG	1A	3021	1/1	0.97	0.10	27,27,27,27	0
56	MG	2A	3413	1/1	0.97	0.15	45,45,45,45	0
56	MG	1A	3119	1/1	0.97	0.22	61,61,61,61	0
56	MG	1a	1604	1/1	0.97	0.12	48,48,48,48	0
56	MG	1A	3824	1/1	0.97	0.89	46,46,46,46	0
56	MG	2a	3015	1/1	0.98	0.10	65,65,65,65	0
56	MG	1A	3737	1/1	0.98	0.16	48,48,48,48	0
56	MG	1A	3738	1/1	0.98	0.36	55,55,55,55	0
56	MG	1A	4034	1/1	0.98	0.09	39,39,39,39	0
56	MG	2A	3679	1/1	0.98	0.08	51,51,51,51	0
56	MG	1A	3205	1/1	0.98	0.22	32,32,32,32	0
56	MG	1A	3275	1/1	0.98	0.12	39,39,39,39	0
56	MG	2A	3682	1/1	0.98	0.19	58,58,58,58	0
56	MG	2A	3312	1/1	0.98	0.44	50,50,50,50	0
56	MG	1A	3011	1/1	0.98	0.20	32,32,32,32	0
56	MG	2A	3685	1/1	0.98	0.18	37,37,37,37	0
56	MG	13	101	1/1	0.98	0.55	43,43,43,43	0
56	MG	2A	3153	1/1	0.98	0.16	68,68,68,68	0
56	MG	1A	3742	1/1	0.98	0.14	32,32,32,32	0
56	MG	1A	3833	1/1	0.98	0.17	38,38,38,38	0
56	MG	1a	1710	1/1	0.98	0.22	58,58,58,58	0
56	MG	1A	3834	1/1	0.98	0.11	45,45,45,45	0
56	MG	1A	3451	1/1	0.98	0.79	27,27,27,27	0
56	MG	15	102	1/1	0.98	0.79	47,47,47,47	0
56	MG	1A	3836	1/1	0.98	0.13	29,29,29,29	0
56	MG	1A	3656	1/1	0.98	0.16	39,39,39,39	0
56	MG	1A	3354	1/1	0.98	0.16	43,43,43,43	0
56	MG	15	106	1/1	0.98	0.62	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	15	107	1/1	0.98	0.10	29,29,29,29	0
56	MG	1A	3511	1/1	0.98	0.10	48,48,48,48	0
56	MG	1A	3145	1/1	0.98	0.10	56,56,56,56	0
56	MG	2A	3167	1/1	0.98	0.16	29,29,29,29	0
56	MG	1B	207	1/1	0.98	0.10	55,55,55,55	0
56	MG	1A	3031	1/1	0.98	0.63	25,25,25,25	0
56	MG	1B	209	1/1	0.98	0.07	48,48,48,48	0
56	MG	2A	3015	1/1	0.98	0.07	44,44,44,44	0
56	MG	1A	3357	1/1	0.98	0.42	39,39,39,39	0
56	MG	1a	1725	1/1	0.98	0.19	36,36,36,36	0
56	MG	1A	3242	1/1	0.98	0.15	58,58,58,58	0
56	MG	1A	3147	1/1	0.98	0.58	41,41,41,41	0
56	MG	2A	3710	1/1	0.98	0.08	48,48,48,48	0
56	MG	2A	3511	1/1	0.98	0.24	70,70,70,70	0
56	MG	2a	3052	1/1	0.98	0.11	54,54,54,54	0
56	MG	1A	3517	1/1	0.98	0.12	45,45,45,45	0
56	MG	1A	3665	1/1	0.98	0.18	34,34,34,34	0
56	MG	2A	3714	1/1	0.98	0.23	55,55,55,55	0
56	MG	1B	216	1/1	0.98	0.17	41,41,41,41	0
56	MG	2a	3057	1/1	0.98	0.26	62,62,62,62	0
56	MG	1A	3178	1/1	0.98	0.51	43,43,43,43	0
56	MG	1A	3459	1/1	0.98	0.28	44,44,44,44	0
56	MG	1A	3948	1/1	0.98	0.17	25,25,25,25	0
56	MG	2A	3344	1/1	0.98	0.14	54,54,54,54	0
56	MG	2A	3519	1/1	0.98	0.14	49,49,49,49	0
56	MG	1A	3850	1/1	0.98	0.14	52,52,52,52	0
56	MG	2a	3064	1/1	0.98	0.07	58,58,58,58	0
56	MG	2A	3722	1/1	0.98	0.13	64,64,64,64	0
56	MG	1A	3361	1/1	0.98	0.29	24,24,24,24	0
56	MG	2A	3522	1/1	0.98	0.13	27,27,27,27	0
56	MG	2A	3523	1/1	0.98	0.39	65,65,65,65	0
56	MG	2A	3726	1/1	0.98	0.17	56,56,56,56	0
56	MG	1A	3590	1/1	0.98	0.08	31,31,31,31	0
56	MG	1A	3282	1/1	0.98	0.19	37,37,37,37	0
56	MG	2A	3031	1/1	0.98	0.37	59,59,59,59	0
56	MG	1a	1738	1/1	0.98	0.10	38,38,38,38	0
56	MG	2A	3351	1/1	0.98	0.19	62,62,62,62	0
56	MG	1B	224	1/1	0.98	0.12	48,48,48,48	0
56	MG	1A	3522	1/1	0.98	0.19	37,37,37,37	0
56	MG	2A	3532	1/1	0.98	0.15	39,39,39,39	0
56	MG	2A	3533	1/1	0.98	0.18	65,65,65,65	0
56	MG	2a	3079	1/1	0.98	0.12	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3760	1/1	0.98	0.13	59,59,59,59	0
56	MG	2A	3036	1/1	0.98	0.16	42,42,42,42	0
56	MG	2A	3192	1/1	0.98	0.15	48,48,48,48	0
56	MG	1A	3245	1/1	0.98	0.37	37,37,37,37	0
56	MG	1A	3095	1/1	0.98	0.12	35,35,35,35	0
56	MG	1a	1744	1/1	0.98	0.33	40,40,40,40	0
56	MG	1A	3859	1/1	0.98	0.10	36,36,36,36	0
56	MG	1A	3150	1/1	0.98	0.15	38,38,38,38	0
56	MG	2a	3088	1/1	0.98	0.10	53,53,53,53	0
56	MG	1A	3526	1/1	0.98	0.31	24,24,24,24	0
56	MG	1A	3862	1/1	0.98	0.15	32,32,32,32	0
56	MG	1D	302	1/1	0.98	0.44	51,51,51,51	0
56	MG	1A	3366	1/1	0.98	0.60	59,59,59,59	0
56	MG	2A	3749	1/1	0.98	0.08	42,42,42,42	0
56	MG	2A	3546	1/1	0.98	0.15	37,37,37,37	0
56	MG	1D	304	1/1	0.98	0.14	42,42,42,42	0
56	MG	2A	3549	1/1	0.98	0.08	35,35,35,35	0
56	MG	1A	3680	1/1	0.98	0.11	22,22,22,22	0
56	MG	2a	3098	1/1	0.98	0.13	70,70,70,70	0
56	MG	2a	3099	1/1	0.98	0.32	55,55,55,55	0
56	MG	2A	3368	1/1	0.98	0.11	49,49,49,49	0
56	MG	1D	306	1/1	0.98	0.77	34,34,34,34	0
56	MG	1a	1754	1/1	0.98	0.09	53,53,53,53	0
56	MG	1D	307	1/1	0.98	0.43	38,38,38,38	0
56	MG	2A	3758	1/1	0.98	0.17	52,52,52,52	0
56	MG	1D	308	1/1	0.98	0.12	47,47,47,47	0
56	MG	1A	3963	1/1	0.98	0.06	41,41,41,41	0
56	MG	2a	3107	1/1	0.98	0.52	61,61,61,61	0
56	MG	1a	1622	1/1	0.98	0.29	55,55,55,55	0
56	MG	1A	3528	1/1	0.98	0.19	23,23,23,23	0
56	MG	1A	3600	1/1	0.98	0.21	29,29,29,29	0
56	MG	1A	3411	1/1	0.98	0.39	61,61,61,61	0
56	MG	1A	3603	1/1	0.98	0.08	54,54,54,54	0
56	MG	1A	3096	1/1	0.98	0.21	43,43,43,43	0
56	MG	2A	3564	1/1	0.98	0.10	49,49,49,49	0
56	MG	2A	3565	1/1	0.98	0.18	47,47,47,47	0
56	MG	1A	3605	1/1	0.98	0.12	27,27,27,27	0
56	MG	1A	3606	1/1	0.98	0.22	40,40,40,40	0
56	MG	1A	3972	1/1	0.98	0.13	64,64,64,64	0
56	MG	2A	3772	1/1	0.98	0.37	46,46,46,46	0
56	MG	1a	1768	1/1	0.98	0.09	39,39,39,39	0
56	MG	2A	3571	1/1	0.98	0.11	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	3250	1/1	0.98	0.10	36,36,36,36	0
56	MG	1A	3874	1/1	0.98	0.08	38,38,38,38	0
56	MG	1a	1772	1/1	0.98	0.09	52,52,52,52	0
56	MG	2A	3778	1/1	0.98	0.27	45,45,45,45	0
56	MG	2A	3068	1/1	0.98	0.75	54,54,54,54	0
56	MG	2A	3390	1/1	0.98	0.12	48,48,48,48	0
56	MG	1A	3414	1/1	0.98	0.21	44,44,44,44	0
56	MG	1a	1634	1/1	0.98	0.21	46,46,46,46	0
56	MG	2A	3783	1/1	0.98	0.17	29,29,29,29	0
56	MG	1A	3111	1/1	0.98	0.36	35,35,35,35	0
56	MG	2A	3227	1/1	0.98	0.10	59,59,59,59	0
56	MG	1A	3778	1/1	0.98	0.14	38,38,38,38	0
56	MG	1A	3779	1/1	0.98	0.06	38,38,38,38	0
56	MG	2A	3788	1/1	0.98	0.15	55,55,55,55	0
56	MG	1A	3003	1/1	0.98	0.14	33,33,33,33	0
56	MG	1F	307	1/1	0.98	0.47	34,34,34,34	0
56	MG	1A	3695	1/1	0.98	0.16	44,44,44,44	0
56	MG	1A	3882	1/1	0.98	0.12	20,20,20,20	0
56	MG	2A	3078	1/1	0.98	0.79	40,40,40,40	0
56	MG	2A	3794	1/1	0.98	0.28	58,58,58,58	0
56	MG	2A	3588	1/1	0.98	0.09	43,43,43,43	0
56	MG	2A	3589	1/1	0.98	0.11	39,39,39,39	0
56	MG	2A	3235	1/1	0.98	0.71	49,49,49,49	0
56	MG	1A	3612	1/1	0.98	0.12	36,36,36,36	0
56	MG	1A	3186	1/1	0.98	0.19	39,39,39,39	0
56	MG	1a	1784	1/1	0.98	0.28	55,55,55,55	0
56	MG	2A	3594	1/1	0.98	0.10	40,40,40,40	0
56	MG	1G	203	1/1	0.98	0.10	51,51,51,51	0
56	MG	2A	3803	1/1	0.98	0.19	39,39,39,39	0
56	MG	2A	3597	1/1	0.98	0.12	37,37,37,37	0
56	MG	1A	3033	1/1	0.98	0.65	26,26,26,26	0
56	MG	1A	3087	1/1	0.98	0.15	27,27,27,27	0
56	MG	1A	3071	1/1	0.98	0.17	43,43,43,43	0
56	MG	2A	3808	1/1	0.98	0.21	46,46,46,46	0
56	MG	2A	3601	1/1	0.98	0.34	45,45,45,45	0
56	MG	1A	3476	1/1	0.98	0.25	41,41,41,41	0
56	MG	1A	3134	1/1	0.98	0.38	36,36,36,36	0
56	MG	2B	201	1/1	0.98	0.09	49,49,49,49	0
56	MG	1P	201	1/1	0.98	0.63	39,39,39,39	0
56	MG	2A	3605	1/1	0.98	0.09	55,55,55,55	0
56	MG	1A	3296	1/1	0.98	0.14	44,44,44,44	0
56	MG	1A	3990	1/1	0.98	0.11	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	1A	3704	1/1	0.98	0.28	41,41,41,41	0
56	MG	2A	3416	1/1	0.98	0.19	68,68,68,68	0
56	MG	1A	3117	1/1	0.98	0.58	47,47,47,47	0
56	MG	1A	3480	1/1	0.98	0.18	57,57,57,57	0
56	MG	1a	1797	1/1	0.98	0.06	58,58,58,58	0
56	MG	2A	3095	1/1	0.98	0.09	47,47,47,47	0
56	MG	1Q	203	1/1	0.98	0.34	43,43,43,43	0
56	MG	1a	1658	1/1	0.98	0.12	52,52,52,52	0
56	MG	1A	3544	1/1	0.98	0.18	42,42,42,42	0
56	MG	2A	3425	1/1	0.98	0.27	31,31,31,31	0
56	MG	1A	3995	1/1	0.98	0.12	47,47,47,47	0
56	MG	1A	3101	1/1	0.98	0.12	37,37,37,37	0
56	MG	1A	3226	1/1	0.98	0.15	41,41,41,41	0
56	MG	1A	3427	1/1	0.98	0.51	56,56,56,56	0
56	MG	1S	201	1/1	0.98	0.17	61,61,61,61	0
56	MG	1A	3079	1/1	0.98	0.60	40,40,40,40	0
56	MG	2A	3432	1/1	0.98	0.11	26,26,26,26	0
56	MG	1A	4000	1/1	0.98	0.08	41,41,41,41	0
56	MG	2A	3106	1/1	0.98	0.13	48,48,48,48	0
56	MG	1A	3163	1/1	0.98	0.19	48,48,48,48	0
56	MG	1A	3430	1/1	0.98	0.24	59,59,59,59	0
56	MG	1A	4003	1/1	0.98	0.24	61,61,61,61	0
56	MG	2a	3186	1/1	0.98	0.12	52,52,52,52	0
56	MG	2A	3630	1/1	0.98	0.13	52,52,52,52	0
56	MG	1A	3339	1/1	0.98	0.41	32,32,32,32	0
56	MG	1A	4005	1/1	0.98	0.17	55,55,55,55	0
56	MG	1A	3432	1/1	0.98	0.17	33,33,33,33	0
56	MG	1A	3555	1/1	0.98	0.14	42,42,42,42	0
56	MG	2O	202	1/1	0.98	0.17	50,50,50,50	0
56	MG	1A	3804	1/1	0.98	0.26	40,40,40,40	0
56	MG	1U	206	1/1	0.98	0.85	34,34,34,34	0
56	MG	1A	4009	1/1	0.98	0.17	26,26,26,26	0
56	MG	2A	3117	1/1	0.98	0.12	49,49,49,49	0
56	MG	1A	3433	1/1	0.98	0.26	37,37,37,37	0
56	MG	1A	3165	1/1	0.98	0.10	30,30,30,30	0
56	MG	2A	3448	1/1	0.98	0.25	54,54,54,54	0
56	MG	1A	3492	1/1	0.98	0.13	45,45,45,45	0
56	MG	1A	3808	1/1	0.98	0.11	55,55,55,55	0
56	MG	1A	3166	1/1	0.98	0.12	33,33,33,33	0
56	MG	2U	201	1/1	0.98	0.23	55,55,55,55	0
56	MG	1A	3436	1/1	0.98	0.20	34,34,34,34	0
56	MG	1A	3267	1/1	0.98	0.14	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3090	1/1	0.98	0.25	50,50,50,50	0
56	MG	2A	3648	1/1	0.98	0.12	41,41,41,41	0
56	MG	1A	4018	1/1	0.98	0.19	27,27,27,27	0
56	MG	2A	3286	1/1	0.98	0.34	57,57,57,57	0
56	MG	2a	3211	1/1	0.98	0.24	66,66,66,66	0
56	MG	2X	102	1/1	0.98	0.21	57,57,57,57	0
56	MG	1A	3439	1/1	0.98	0.90	44,44,44,44	0
56	MG	2A	3130	1/1	0.98	0.15	32,32,32,32	0
56	MG	1W	203	1/1	0.98	0.33	36,36,36,36	0
56	MG	20	103	1/1	0.98	0.10	52,52,52,52	0
56	MG	1A	3001	1/1	0.98	0.14	39,39,39,39	0
56	MG	1A	3169	1/1	0.98	0.15	22,22,22,22	0
56	MG	2A	3657	1/1	0.98	0.11	36,36,36,36	0
56	MG	1A	3643	1/1	0.98	0.13	32,32,32,32	0
56	MG	1A	3728	1/1	0.98	0.26	57,57,57,57	0
56	MG	26	101	1/1	0.98	0.32	53,53,53,53	0
56	MG	1A	3346	1/1	0.98	0.14	40,40,40,40	0
56	MG	2A	3295	1/1	0.98	0.28	52,52,52,52	0
56	MG	2A	3296	1/1	0.98	0.17	54,54,54,54	0
56	MG	1t	201	1/1	0.98	0.32	55,55,55,55	0
56	MG	1A	3501	1/1	0.98	0.15	22,22,22,22	0
56	MG	1A	3073	1/1	0.98	0.31	41,41,41,41	0
56	MG	2A	3666	1/1	0.98	0.11	44,44,44,44	0
56	MG	2A	3470	1/1	0.98	0.09	66,66,66,66	0
56	MG	1A	3348	1/1	0.98	0.50	38,38,38,38	0
56	MG	1A	3141	1/1	0.98	0.12	43,43,43,43	0
56	MG	2A	3303	1/1	0.98	0.05	67,67,67,67	0
56	MG	1A	3142	1/1	0.98	0.25	43,43,43,43	0
57	ZN	16	103	1/1	0.98	0.21	41,41,41,41	0
57	ZN	1n	103	1/1	0.98	0.11	70,70,70,70	0
56	MG	1A	3573	1/1	0.98	0.15	35,35,35,35	0
57	ZN	26	102	1/1	0.98	0.23	62,62,62,62	0
56	MG	1A	4031	1/1	0.98	0.17	47,47,47,47	0
56	MG	2A	3478	1/1	0.98	0.09	56,56,56,56	0
56	MG	2A	3675	1/1	0.98	0.51	70,70,70,70	0
56	MG	1U	202	1/1	0.99	0.35	43,43,43,43	0
56	MG	1A	3558	1/1	0.99	0.20	47,47,47,47	0
56	MG	1A	3230	1/1	0.99	0.34	55,55,55,55	0
56	MG	1a	1665	1/1	0.99	0.14	60,60,60,60	0
56	MG	1A	3668	1/1	0.99	0.27	45,45,45,45	0
56	MG	1A	3593	1/1	0.99	0.17	44,44,44,44	0
56	MG	1A	3131	1/1	0.99	0.51	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	3112	1/1	0.99	0.20	51,51,51,51	0
56	MG	1A	3858	1/1	0.99	0.17	27,27,27,27	0
56	MG	1A	3672	1/1	0.99	0.16	37,37,37,37	0
56	MG	2A	3298	1/1	0.99	0.08	66,66,66,66	0
56	MG	1A	3967	1/1	0.99	0.10	50,50,50,50	0
56	MG	2A	3529	1/1	0.99	0.10	51,51,51,51	0
56	MG	2A	3374	1/1	0.99	0.09	37,37,37,37	0
56	MG	1V	202	1/1	0.99	0.15	41,41,41,41	0
56	MG	2A	3376	1/1	0.99	0.15	45,45,45,45	0
56	MG	1A	3211	1/1	0.99	0.17	40,40,40,40	0
56	MG	1A	3151	1/1	0.99	0.16	44,44,44,44	0
56	MG	1A	3811	1/1	0.99	0.19	56,56,56,56	0
56	MG	1A	3283	1/1	0.99	0.16	41,41,41,41	0
56	MG	1E	302	1/1	0.99	0.42	47,47,47,47	0
56	MG	1A	3194	1/1	0.99	0.15	36,36,36,36	0
56	MG	1A	3164	1/1	0.99	0.15	40,40,40,40	0
56	MG	1A	3678	1/1	0.99	0.12	39,39,39,39	0
56	MG	2A	3025	1/1	0.99	0.09	44,44,44,44	0
56	MG	1A	3601	1/1	0.99	0.10	33,33,33,33	0
56	MG	1A	3868	1/1	0.99	0.20	46,46,46,46	0
56	MG	1A	3082	1/1	0.99	0.11	39,39,39,39	0
56	MG	1X	103	1/1	0.99	0.14	34,34,34,34	0
56	MG	1A	3013	1/1	0.99	0.33	41,41,41,41	0
56	MG	1A	3449	1/1	0.99	0.26	58,58,58,58	0
56	MG	2A	3548	1/1	0.99	0.14	43,43,43,43	0
56	MG	1A	3772	1/1	0.99	0.14	34,34,34,34	0
56	MG	2a	3187	1/1	0.99	0.20	47,47,47,47	0
56	MG	1A	3421	1/1	0.99	0.19	44,44,44,44	0
56	MG	1A	3684	1/1	0.99	0.08	43,43,43,43	0
56	MG	2A	3552	1/1	0.99	0.06	50,50,50,50	0
56	MG	2A	3472	1/1	0.99	0.18	62,62,62,62	0
56	MG	1A	3729	1/1	0.99	0.19	37,37,37,37	0
56	MG	1A	3181	1/1	0.99	0.59	48,48,48,48	0
56	MG	1A	3127	1/1	0.99	0.53	50,50,50,50	0
56	MG	1A	3878	1/1	0.99	0.09	43,43,43,43	0
56	MG	1a	1758	1/1	0.99	0.10	54,54,54,54	0
56	MG	1B	201	1/1	0.99	0.19	56,56,56,56	0
56	MG	2A	3041	1/1	0.99	0.08	35,35,35,35	0
56	MG	1A	3687	1/1	0.99	0.19	45,45,45,45	0
56	MG	1A	3608	1/1	0.99	0.21	42,42,42,42	0
56	MG	2A	3254	1/1	0.99	0.32	42,42,42,42	0
56	MG	2A	3731	1/1	0.99	0.18	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3183	1/1	0.99	0.38	50,50,50,50	0
56	MG	1A	3690	1/1	0.99	0.16	44,44,44,44	0
56	MG	2A	3649	1/1	0.99	0.35	49,49,49,49	0
56	MG	1A	3574	1/1	0.99	0.18	50,50,50,50	0
56	MG	2A	3567	1/1	0.99	0.13	52,52,52,52	0
56	MG	1A	3831	1/1	0.99	0.09	33,33,33,33	0
56	MG	1A	3265	1/1	0.99	0.19	36,36,36,36	0
56	MG	1A	3266	1/1	0.99	0.23	40,40,40,40	0
56	MG	2A	3489	1/1	0.99	0.36	55,55,55,55	0
56	MG	1A	3372	1/1	0.99	0.19	42,42,42,42	0
56	MG	2A	3119	1/1	0.99	0.16	46,46,46,46	0
56	MG	1a	1769	1/1	0.99	0.14	30,30,30,30	0
56	MG	1A	3144	1/1	0.99	0.38	42,42,42,42	0
56	MG	1A	3202	1/1	0.99	0.52	37,37,37,37	0
56	MG	1A	3547	1/1	0.99	0.12	42,42,42,42	0
56	MG	1A	3548	1/1	0.99	0.20	51,51,51,51	0
56	MG	1B	215	1/1	0.99	0.10	44,44,44,44	0
56	MG	1A	3655	1/1	0.99	0.16	42,42,42,42	0
56	MG	1A	3946	1/1	0.99	0.08	35,35,35,35	0
56	MG	1A	3034	1/1	0.99	0.60	45,45,45,45	0
56	MG	1A	3223	1/1	0.99	0.34	42,42,42,42	0
56	MG	2A	3273	1/1	0.99	0.13	71,71,71,71	0
56	MG	2A	3131	1/1	0.99	0.17	36,36,36,36	0
56	MG	1A	3105	1/1	0.99	0.12	42,42,42,42	0
56	MG	1A	3225	1/1	0.99	0.27	49,49,49,49	0
56	MG	1A	3844	1/1	0.99	0.41	53,53,53,53	0
56	MG	1A	3158	1/1	0.99	0.49	39,39,39,39	0
56	MG	2A	3206	1/1	0.99	0.19	55,55,55,55	0
56	MG	2P	201	1/1	0.99	0.23	53,53,53,53	0
56	MG	1A	3249	1/1	0.99	0.15	26,26,26,26	0
56	MG	1A	3069	1/1	0.99	0.14	28,28,28,28	0
57	ZN	1Y	202	1/1	0.99	0.20	65,65,65,65	0
56	MG	2A	3067	1/1	0.99	0.26	46,46,46,46	0
56	MG	1a	1657	1/1	0.99	0.12	58,58,58,58	0
57	ZN	19	103	1/1	0.99	0.16	44,44,44,44	0
56	MG	2A	3595	1/1	0.99	0.30	57,57,57,57	0
57	ZN	2Y	202	1/1	0.99	0.17	79,79,79,79	0
56	MG	2R	203	1/1	0.99	0.17	39,39,39,39	0
57	ZN	25	105	1/1	0.99	0.22	58,58,58,58	0
56	MG	1A	3173	1/1	0.99	0.15	41,41,41,41	0
56	MG	1A	3799	1/1	0.99	0.30	36,36,36,36	0
56	MG	1A	3148	1/1	0.99	0.28	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	SF4	1d	501	8/8	0.99	0.18	64,70,81,85	0
58	SF4	2d	302	8/8	0.99	0.19	63,75,80,93	0
56	MG	1A	3627	1/1	0.99	0.11	31,31,31,31	0
56	MG	1A	3483	1/1	1.00	0.29	37,37,37,37	0
56	MG	2A	3128	1/1	1.00	0.14	34,34,34,34	0
56	MG	1A	3328	1/1	1.00	0.13	39,39,39,39	0
57	ZN	15	108	1/1	1.00	0.19	40,40,40,40	0

6.5 Other polymers (i)

There are no such residues in this entry.