Full wwPDB X-ray Structure Validation Report (i)

Nov 6, 2023 – 12:50 AM EST

PDB ID	:	8CVJ
Title	:	Crystal structure of the Thermus thermophilus 70S ribosome in complex with mRNA, aminoacylated A-site Phe-NH-tRNAphe, peptidyl P-site fMSEAC-NH-tRNAmet, and deacylated E-site tRNAphe at 2.40A resolution
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Deposited on	:	2022-05-18
Resolution	:	2.40 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 (i) 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 (i)) were used in the production of this report:

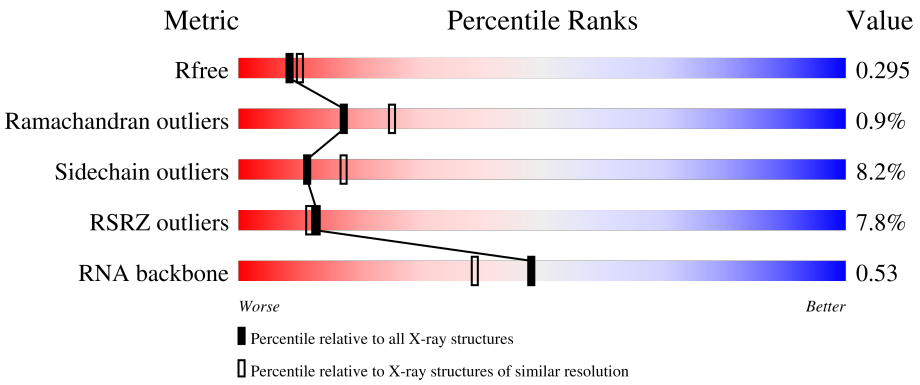
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.40 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	3907 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)
RNA backbone	3102	1174 (2.80-2.00)

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	5% 82% 16% • •
1	2A	2915	5% 79% 16% •
2	1B	121	88% 12% •
2	2B	121	2% 79% 21% •
3	1D	276	% 96% •

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Mol	Chain	Length	Quality of chain
3	2D	276	%, 95%
4	1E	206	95%
4	2E	206	%, 94%, 5%
5	1F	210	2%, 89%, 8%
5	2F	210	4%, 89%, 7%
6	1G	182	%, 93%, 6%
6	2G	182	7%, 88%, 10%
7	1H	180	90%, 7%
7	2H	180	41%, 88%, 8%
8	1I	148	%, 86%, 12%
8	2I	148	13%, 84%, 14%
9	1N	140	96%
9	2N	140	%, 96%
10	1O	122	98%
10	2O	122	%, 98%
11	1P	150	%, 91%, 9%
11	2P	150	10%, 90%, 9%
12	1Q	141	%, 96%
12	2Q	141	3%, 96%
13	1R	118	96%
13	2R	118	%, 97%
14	1S	112	95%
14	2S	112	11%, 88%, 9%
15	1T	146	86%, 10%
15	2T	146	3%, 81%, 9%, 10%

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Mol	Chain	Length	Quality of chain
16	1U	118	92% 5%
16	2U	118	3% 96%
17	1V	101	94% 5%
17	2V	101	% 96%
18	1W	113	94% 5%
18	2W	113	96%
19	1X	96	2% 96%
19	2X	96	7% 94% 5%
20	1Y	110	% 92% 5%
20	2Y	110	9% 92% 5%
21	1Z	206	7% 68% 6% 25%
21	2Z	206	18% 70% 8% 22%
22	10	85	% 98%
22	20	85	4% 95%
23	11	98	% 92% 6%
23	21	98	2% 92% 7%
24	12	72	93%
24	22	72	7% 89% 8%
25	13	60	90% 8%
25	23	60	2% 93% 5%
26	14	71	13% 80% 14%
26	24	71	25% 75% 21%
27	15	60	2% 87% 12%
27	25	60	92% 7%
28	16	54	87% 11%

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Mol	Chain	Length	Quality of chain
28	26	54	7% 85% 13%
29	17	49	2% 92% 6%
29	27	49	6% 90% 8%
30	18	65	92% 6%
30	28	65	2% 92% 6%
31	19	37	95% 5%
31	29	37	14% 100%
32	1a	1521	6% 81% 17%
32	2a	1521	10% 80% 18%
33	1b	256	15% 79% 11% 10%
33	2b	256	29% 78% 12% 10%
34	1c	239	5% 81% 5% 14%
34	2c	239	16% 79% 7% 14%
35	1d	209	% 90% 10%
35	2d	209	5% 93% 7%
36	1e	162	2% 86% 5% 9%
36	2e	162	9% 86% 5% 9%
37	1f	101	93% 6%
37	2f	101	92% 7%
38	1g	156	4% 89% 10%
38	2g	156	21% 89% 10%
39	1h	138	3% 93% 7%
39	2h	138	9% 91% 7%
40	1i	128	24% 90% 9%
40	2i	128	66% 90% 9%

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Mol	Chain	Length	Quality of chain
41	1j	105	20% 83% 10% 8%
41	2j	105	40% 81% 10% 9%
42	1k	129	3% 79% 9% 12%
42	2k	129	4% 82% 6% 12%
43	1l	132	88% 5% 8%
43	2l	132	84% 8% 8%
44	1m	126	5% 88% 10%
44	2m	126	12% 85% 11%
45	1n	61	16% 89% 10%
45	2n	61	51% 93% 5%
46	1o	89	91% 8%
46	2o	89	3% 93% 6%
47	1p	88	11% 86% 7% 7%
47	2p	88	8% 89% 5% 7%
48	1q	105	9% 89% 6% 6%
48	2q	105	16% 86% 9% 6%
49	1r	88	5% 70% 7% 23%
49	2r	88	2% 68% 9% 23%
50	1s	93	3% 82% 8% 11%
50	2s	93	14% 80% 10% 11%
51	1t	106	24% 83% 8% 9%
51	2t	106	25% 86% 5% 9%
52	1u	27	19% 78% 7% 15%
52	2u	27	48% 85% 15%
53	1v	24	12% 54% 46%

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Mol	Chain	Length	Quality of chain
53	2v	24	21% 54% 46%
54	1w	76	9% 61% 33%
54	2w	76	12% 57% 36% 5%
55	1x	77	78% 22%
55	2x	77	75% 25%
56	1z	5	80% 20%
56	2z	5	60% 40%
57	1y	76	76% 53% 39% 5%
57	2y	76	75% 61% 33%

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
57	MIA	1y	37	-	-	-	X
57	PSU	1y	55	-	-	-	X
57	MIA	2y	37	-	-	-	X
57	PSU	2y	39	-	-	-	X
57	PSU	2y	55	-	-	-	X
58	MG	2A	3223	-	-	-	X
58	MG	2A	3864	-	-	-	X

2 Entry composition (i)

There are 62 unique types of molecules in this entry. The entry contains 299959 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
			Total	C	N	O	P			
1	1A	2871	61852	27531	11572	19878	2871	0	0	0
1	2A	2800	60322	26848	11284	19390	2800	0	0	0

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	1F	202	1583	1009	297	275	2	0	0	0
5	2F	202	1579	1007	296	274	2	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 53 is a RNA chain called MF-mRNA.

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

- Molecule 54 is a RNA chain called A-site Aminoacyl-tRNA Phe-NH-tRNAphe.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
54	1w	74	1603	722	287	518	74	2	0	0	0
54	2w	72	1555	699	280	502	72	2	0	0	0

- Molecule 55 is a RNA chain called P-site Peptidyl-tRNA fMSEAC-NH-tRNAmet RNA-part.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
55	1x	77	1646	734	298	536	77	1	0	0	0
55	2x	77	1646	734	298	536	77	1	0	0	0

- Molecule 56 is a protein called P-site Peptidyl-tRNA fMSEAC-NH-tRNAmet Peptide-part.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
56	1z	4	26	14	4	7	1	0	0	0
56	2z	3	20	11	3	5	1	0	0	0

- Molecule 57 is a RNA chain called E-site Deacylated tRNAphe.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
57	1y	74	1585	707	285	518	74	1	0	0	0
57	2y	73	1565	698	283	510	73	1	0	0	0

- Molecule 58 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
58	1A	1108	1108	1108	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
58	1B	38	38	38	0	0
58	1D	10	10	10	0	0
58	1E	14	14	14	0	0
58	1F	14	14	14	0	0
58	1G	5	5	5	0	0
58	1H	1	1	1	0	0
58	1I	1	1	1	0	0
58	1N	5	5	5	0	0
58	1O	5	5	5	0	0
58	1P	4	4	4	0	0
58	1Q	8	8	8	0	0
58	1R	3	3	3	0	0
58	1S	3	3	3	0	0
58	1T	3	3	3	0	0
58	1U	11	11	11	0	0
58	1V	6	6	6	0	0
58	1W	4	4	4	0	0
58	1X	6	6	6	0	0
58	1Y	3	3	3	0	0
58	1Z	3	3	3	0	0
58	10	7	7	7	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
58	11	6	6	6	0	0
58	12	2	2	2	0	0
58	13	6	6	6	0	0
58	14	1	1	1	0	0
58	15	7	7	7	0	0
58	16	2	2	2	0	0
58	17	5	5	5	0	0
58	18	5	5	5	0	0
58	19	1	1	1	0	0
58	1a	213	213	213	0	0
58	1b	1	1	1	0	0
58	1d	1	1	1	0	0
58	1e	2	2	2	0	0
58	1f	2	2	2	0	0
58	1k	1	1	1	0	0
58	1l	2	2	2	0	0
58	1m	1	1	1	0	0
58	1n	2	2	2	0	0
58	1t	1	1	1	0	0
58	1v	1	1	1	0	0
58	1w	9	9	9	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
58	1x	12	12	12	0	0
58	2A	869	869	869	0	0
58	2B	19	19	19	0	0
58	2D	7	7	7	0	0
58	2E	8	8	8	0	0
58	2F	6	6	6	0	0
58	2G	1	1	1	0	0
58	2O	1	1	1	0	0
58	2P	1	1	1	0	0
58	2Q	2	2	2	0	0
58	2R	2	2	2	0	0
58	2T	3	3	3	0	0
58	2U	2	2	2	0	0
58	2V	2	2	2	0	0
58	2W	2	2	2	0	0
58	2X	2	2	2	0	0
58	2Y	1	1	1	0	0
58	2Z	1	1	1	0	0
58	20	3	3	3	0	0
58	21	1	1	1	0	0
58	23	3	3	3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
58	25	6	6	6	0	0
58	27	3	3	3	0	0
58	28	3	3	3	0	0
58	2a	235	235	235	0	0
58	2d	2	2	2	0	0
58	2e	1	1	1	0	0
58	2f	2	2	2	0	0
58	2g	1	1	1	0	0
58	2i	1	1	1	0	0
58	2j	1	1	1	0	0
58	2k	1	1	1	0	0
58	2l	4	4	4	0	0
58	2n	1	1	1	0	0
58	2p	1	1	1	0	0
58	2q	2	2	2	0	0
58	2r	1	1	1	0	0
58	2t	1	1	1	0	0
58	2v	4	4	4	0	0
58	2w	4	4	4	0	0
58	2x	6	6	6	0	0
58	2y	1	1	1	0	0

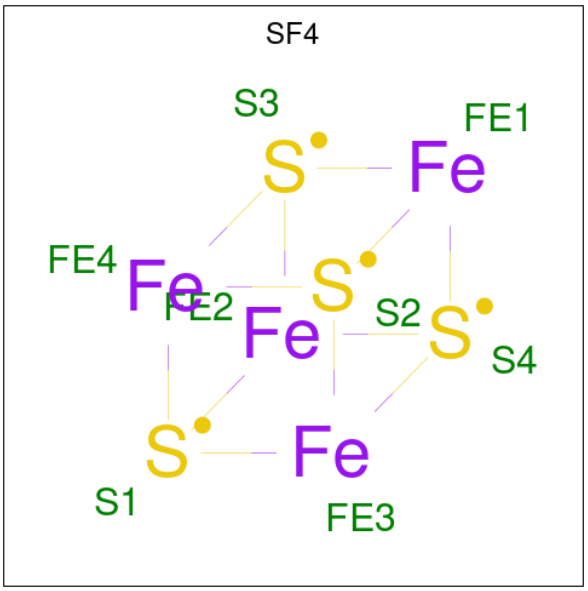
- Molecule 59 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	1Y	1	Total Zn 1 1	0	0
60	14	1	Total Zn 1 1	0	0
60	15	1	Total Zn 1 1	0	0
60	16	1	Total Zn 1 1	0	0
60	19	1	Total Zn 1 1	0	0
60	1n	1	Total Zn 1 1	0	0
60	2Y	1	Total Zn 1 1	0	0
60	24	1	Total Zn 1 1	0	0
60	25	1	Total Zn 1 1	0	0
60	26	1	Total Zn 1 1	0	0
60	29	1	Total Zn 1 1	0	0
60	2n	1	Total Zn 1 1	0	0

- Molecule 61 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1d	1	Total Fe S 8 4 4	0	0
61	2d	1	Total Fe S 8 4 4	0	0

- Molecule 62 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	1A	1956	Total O 1956 1956	0	0
62	1B	62	Total O 62 62	0	0
62	1D	27	Total O 27 27	0	0
62	1E	28	Total O 28 28	0	0
62	1F	22	Total O 22 22	0	0
62	1G	3	Total O 3 3	0	0
62	1H	2	Total O 2 2	0	0
62	1N	4	Total O 4 4	0	0
62	1O	5	Total O 5 5	0	0
62	1P	21	Total O 21 21	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	1Q	6	Total O 6 6	0	0
62	1R	11	Total O 11 11	0	0
62	1S	4	Total O 4 4	0	0
62	1T	7	Total O 7 7	0	0
62	1U	11	Total O 11 11	0	0
62	1V	8	Total O 8 8	0	0
62	1W	8	Total O 8 8	0	0
62	1X	5	Total O 5 5	0	0
62	1Y	3	Total O 3 3	0	0
62	1Z	1	Total O 1 1	0	0
62	10	13	Total O 13 13	0	0
62	11	12	Total O 12 12	0	0
62	12	3	Total O 3 3	0	0
62	13	4	Total O 4 4	0	0
62	14	1	Total O 1 1	0	0
62	15	6	Total O 6 6	0	0
62	16	2	Total O 2 2	0	0
62	17	10	Total O 10 10	0	0
62	18	8	Total O 8 8	0	0
62	1a	326	Total O 326 326	0	0
62	1b	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	1e	1	Total O 1 1	0	0
62	1f	1	Total O 1 1	0	0
62	1g	1	Total O 1 1	0	0
62	1i	1	Total O 1 1	0	0
62	1l	4	Total O 4 4	0	0
62	1m	1	Total O 1 1	0	0
62	1o	1	Total O 1 1	0	0
62	1p	1	Total O 1 1	0	0
62	1q	2	Total O 2 2	0	0
62	1u	1	Total O 1 1	0	0
62	1v	5	Total O 5 5	0	0
62	1w	8	Total O 8 8	0	0
62	1x	9	Total O 9 9	0	0
62	1z	1	Total O 1 1	0	0
62	1y	1	Total O 1 1	0	0
62	2A	1067	Total O 1067 1067	0	0
62	2B	22	Total O 22 22	0	0
62	2D	26	Total O 26 26	0	0
62	2E	17	Total O 17 17	0	0
62	2F	13	Total O 13 13	0	0
62	2N	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	2O	1	Total O 1 1	0	0
62	2P	10	Total O 10 10	0	0
62	2Q	2	Total O 2 2	0	0
62	2R	4	Total O 4 4	0	0
62	2T	4	Total O 4 4	0	0
62	2U	2	Total O 2 2	0	0
62	2W	2	Total O 2 2	0	0
62	2X	4	Total O 4 4	0	0
62	2Y	1	Total O 1 1	0	0
62	2Z	1	Total O 1 1	0	0
62	20	3	Total O 3 3	0	0
62	21	10	Total O 10 10	0	0
62	22	1	Total O 1 1	0	0
62	23	1	Total O 1 1	0	0
62	25	2	Total O 2 2	0	0
62	27	4	Total O 4 4	0	0
62	28	3	Total O 3 3	0	0
62	29	1	Total O 1 1	0	0
62	2a	225	Total O 225 225	0	0
62	2c	1	Total O 1 1	0	0
62	2d	1	Total O 1 1	0	0

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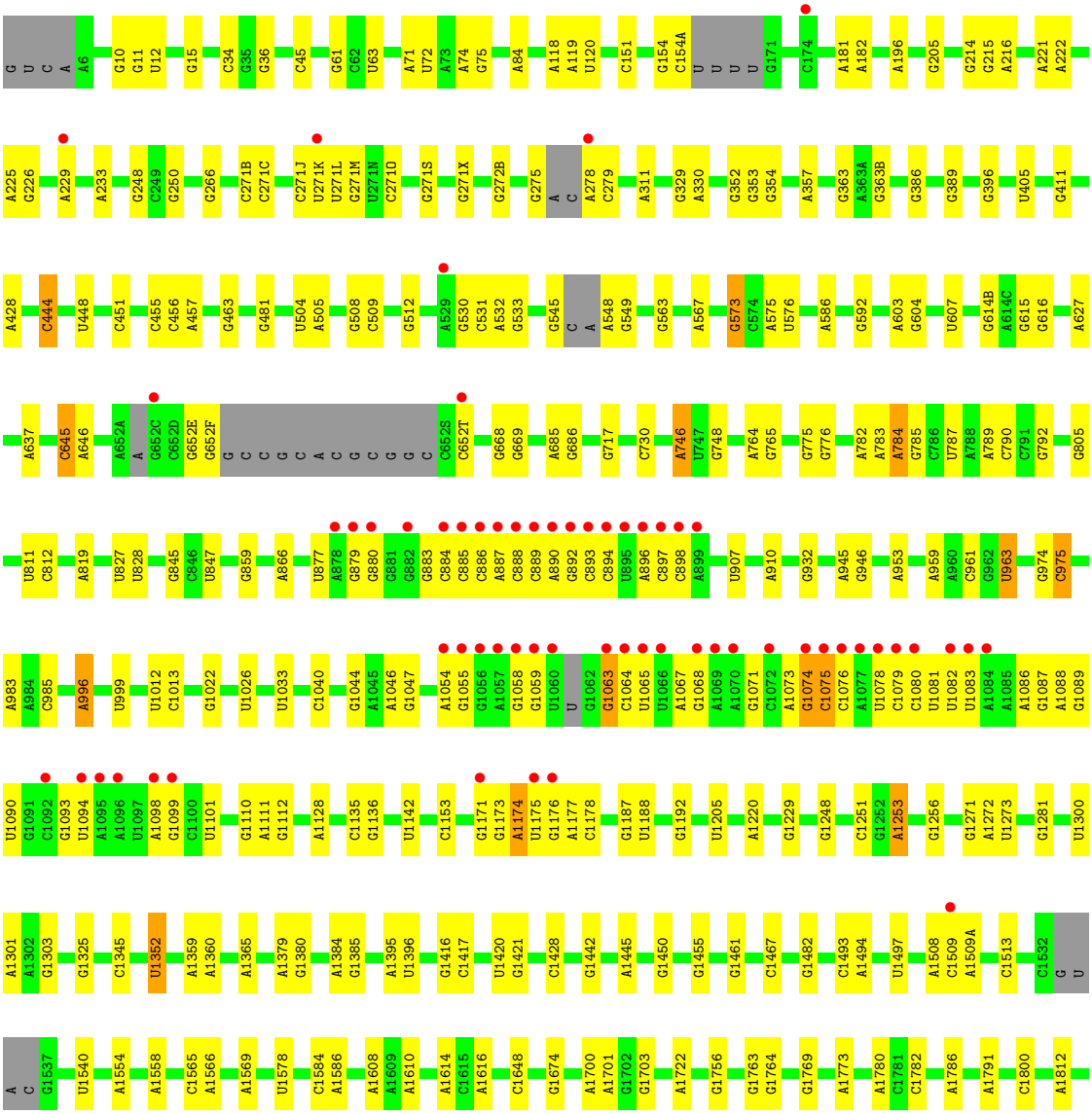
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	2e	2	Total O 2 2	0	0
62	2i	1	Total O 1 1	0	0
62	2j	3	Total O 3 3	0	0
62	2l	6	Total O 6 6	0	0
62	2p	2	Total O 2 2	0	0
62	2r	1	Total O 1 1	0	0
62	2t	2	Total O 2 2	0	0
62	2v	1	Total O 1 1	0	0
62	2w	5	Total O 5 5	0	0
62	2x	3	Total O 3 3	0	0
62	2z	1	Total O 1 1	0	0

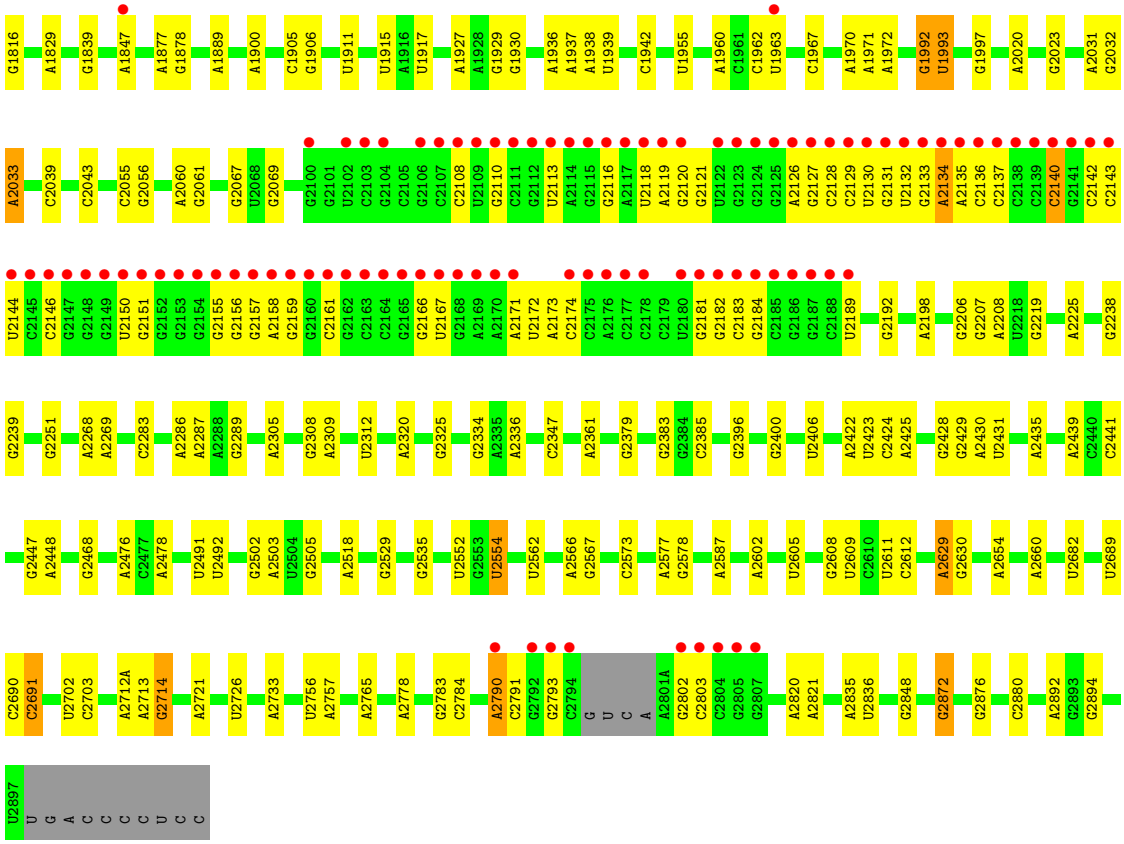
3 Residue-property plots (i)

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

- Molecule 1: 23S Ribosomal RNA

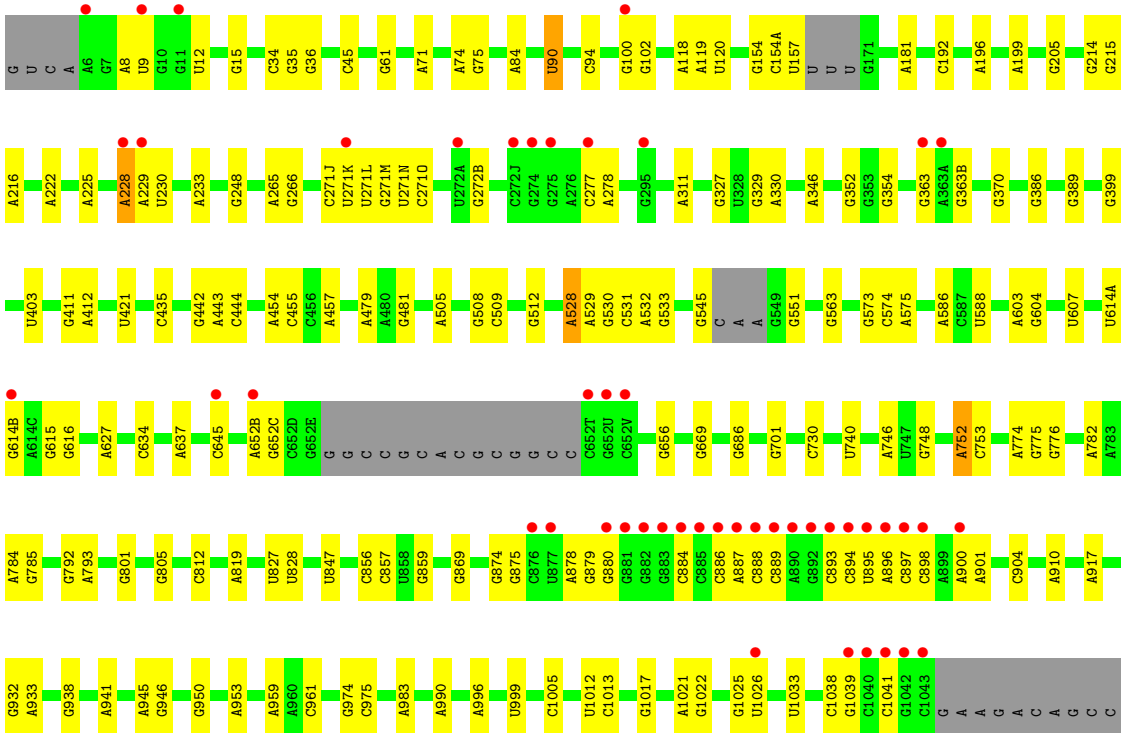
Chain 1A:

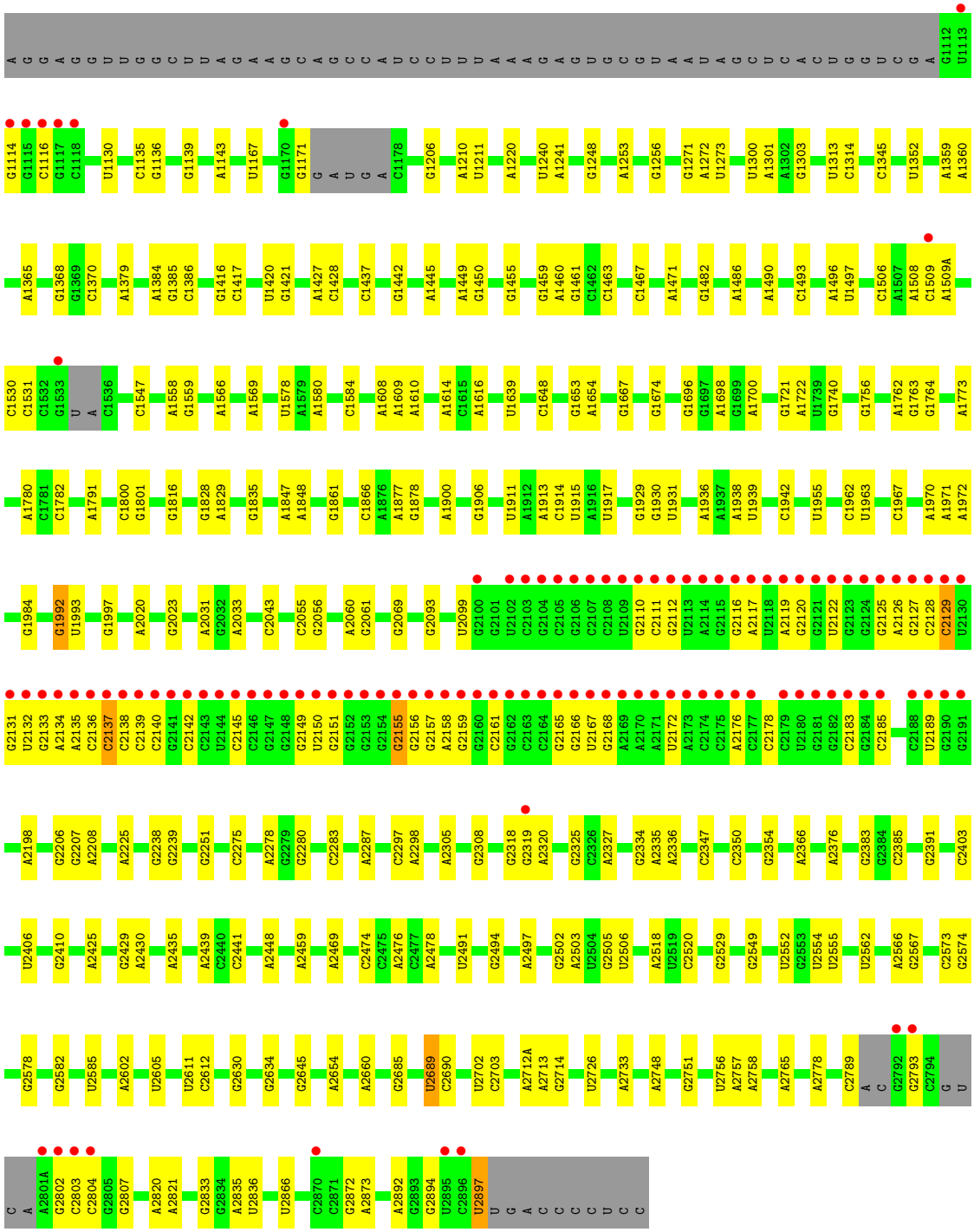




• Molecule 1: 23S Ribosomal RNA

Chain 2A:



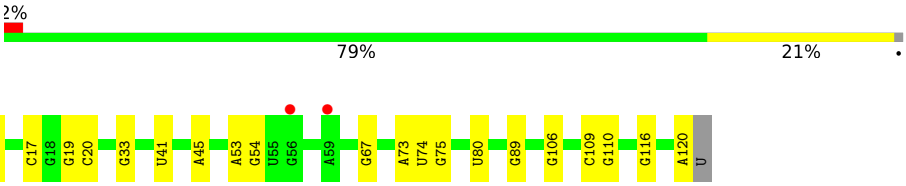


- Molecule 2: 5S Ribosomal RNA

Chain 1B:

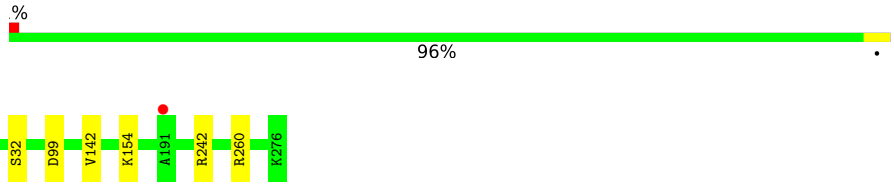
- Molecule 2: 5S Ribosomal RNA

Chain 2B:



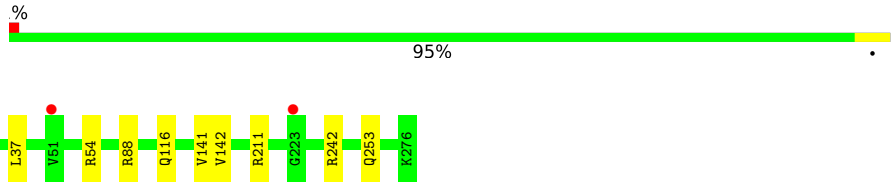
• Molecule 3: 50S ribosomal protein L2

Chain 1D:



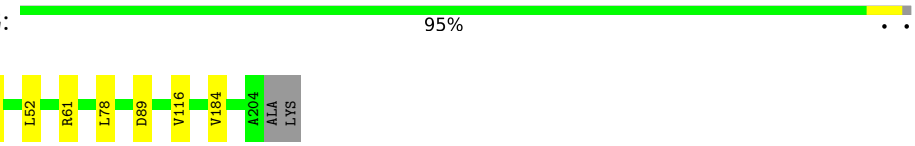
• Molecule 3: 50S ribosomal protein L2

Chain 2D:



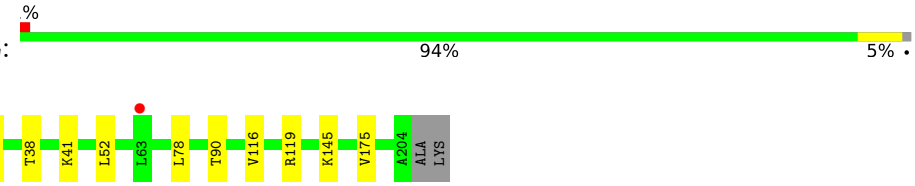
• Molecule 4: 50S ribosomal protein L3

Chain 1E:



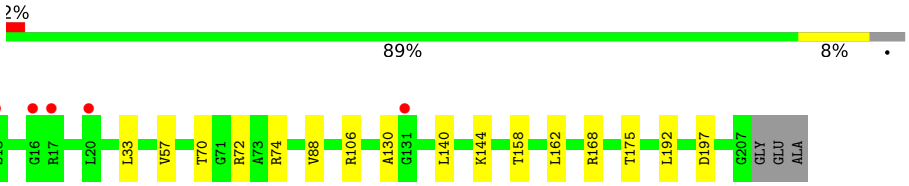
• Molecule 4: 50S ribosomal protein L3

Chain 2E:



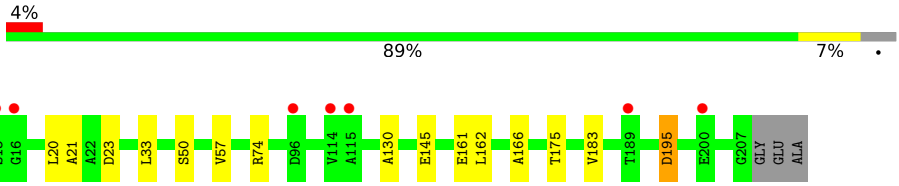
• Molecule 5: 50S ribosomal protein L4

Chain 1F:



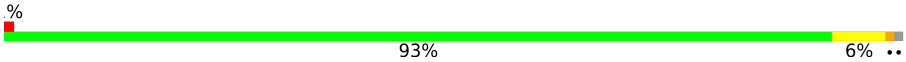
• Molecule 5: 50S ribosomal protein L4

Chain 2F:



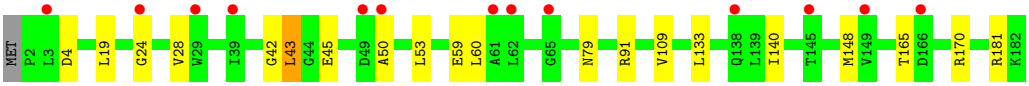
• Molecule 6: 50S ribosomal protein L5

Chain 1G:



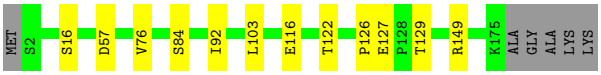
• Molecule 6: 50S ribosomal protein L5

Chain 2G:



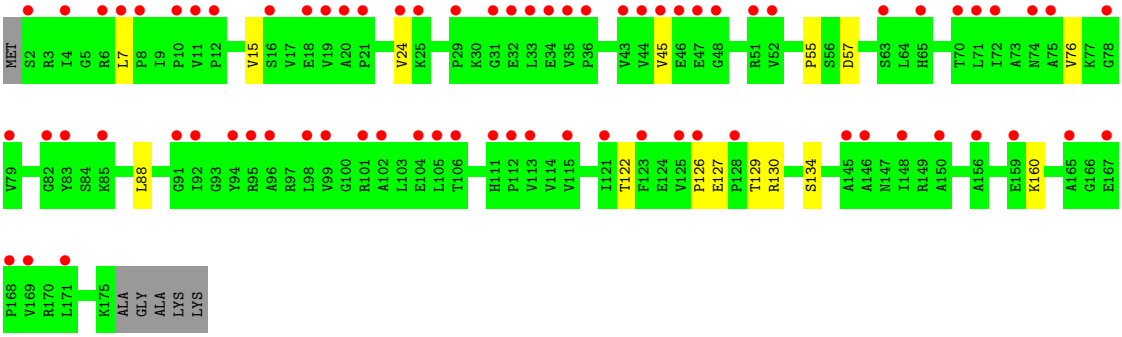
• Molecule 7: 50S ribosomal protein L6

Chain 1H:



• Molecule 7: 50S ribosomal protein L6

Chain 2H:

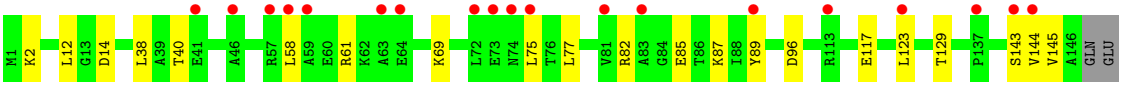


• Molecule 8: 50S ribosomal protein L9

Chain 1I:

• Molecule 8: 50S ribosomal protein L9

Chain 2I:



• Molecule 9: 50S ribosomal protein L13

Chain 1N: 96%

M1 K2 V9 T28 V46 A47 M48 I71 V140

• Molecule 9: 50S ribosomal protein L13

Chain 2N: % 96%

M1 K2 V9 E10 T28 M48 T73 K83 V140

• Molecule 10: 50S ribosomal protein L14

Chain 1O: 98%

M1 S28 L106 M112 L122

• Molecule 10: 50S ribosomal protein L14

Chain 2O: % 98%

M1 Y32 T96 E108 S116 L122

• Molecule 11: 50S ribosomal protein L15

Chain 1P: % 91% 9%

M1 K2 L3 R7 K29 Q38 G44 L45 K86 E92 T96 P97 E98 V101 I114 S133 L147 L148 E149 ALA

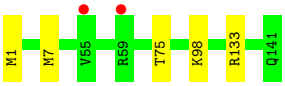
• Molecule 11: 50S ribosomal protein L15

Chain 2P: 10% 90% 9%

M1 K2 L3 R7 G22 K29 K36 G37 Q38 G44 L45 T58 K86 F91 E92 G93 E94 V95 T96 P97 E98 V101 R102 A103 G109 Y110 P122 S133 A134 L135 L138 L148 E149 ALA

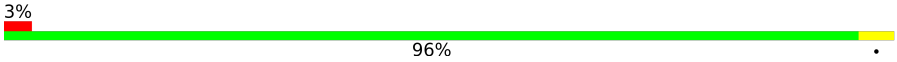
• Molecule 12: 50S ribosomal protein L16

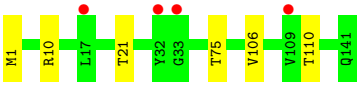
Chain 1Q: % 96%



• Molecule 12: 50S ribosomal protein L16

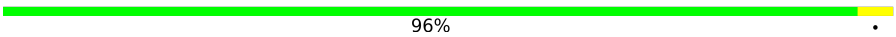
Chain 2Q:

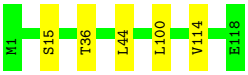




• Molecule 13: 50S ribosomal protein L17

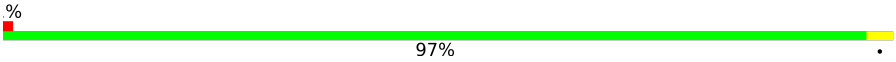
Chain 1R:

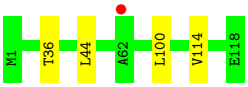




• Molecule 13: 50S ribosomal protein L17

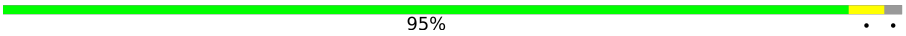
Chain 2R:

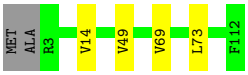




• Molecule 14: 50S ribosomal protein L18

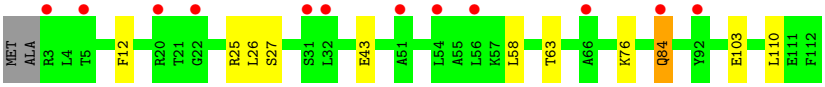
Chain 1S:





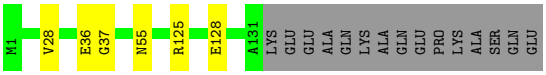
• Molecule 14: 50S ribosomal protein L18

Chain 2S:



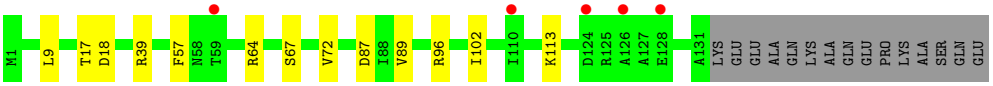
• Molecule 15: 50S ribosomal protein L19

Chain 1T:



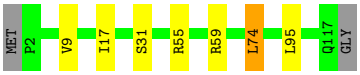
• Molecule 15: 50S ribosomal protein L19

Chain 2T:



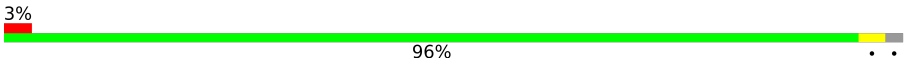
• Molecule 16: 50S ribosomal protein L20

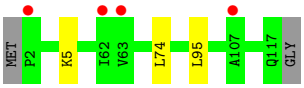
Chain 1U:



• Molecule 16: 50S ribosomal protein L20

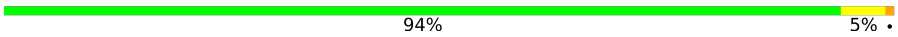
Chain 2U:





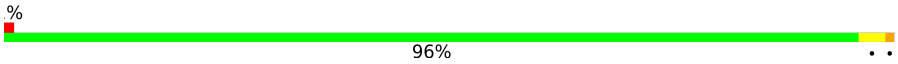
• Molecule 17: 50S ribosomal protein L21

Chain 1V:



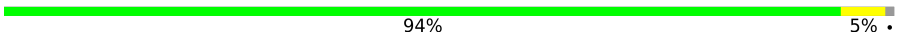
• Molecule 17: 50S ribosomal protein L21

Chain 2V:



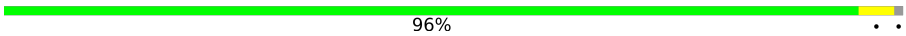
• Molecule 18: 50S ribosomal protein L22

Chain 1W:



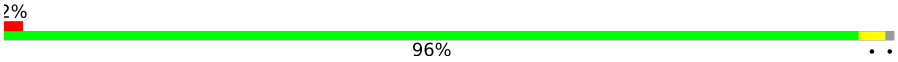
• Molecule 18: 50S ribosomal protein L22

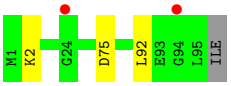
Chain 2W:



• Molecule 19: 50S ribosomal protein L23

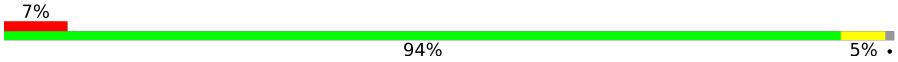
Chain 1X:

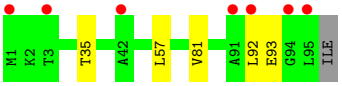




• Molecule 19: 50S ribosomal protein L23

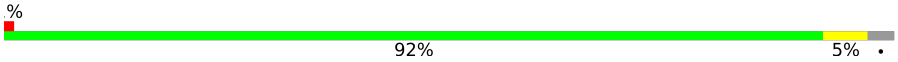
Chain 2X:

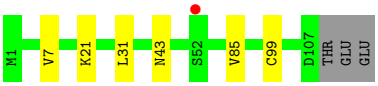




• Molecule 20: 50S ribosomal protein L24

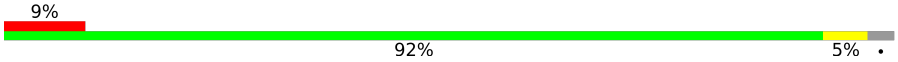
Chain 1Y:

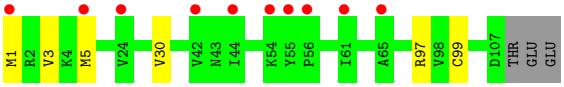




• Molecule 20: 50S ribosomal protein L24

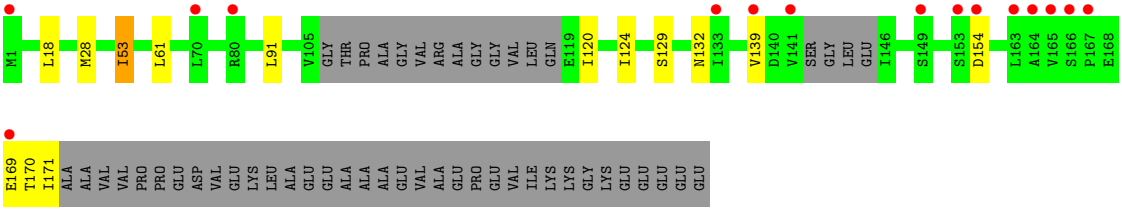
Chain 2Y:





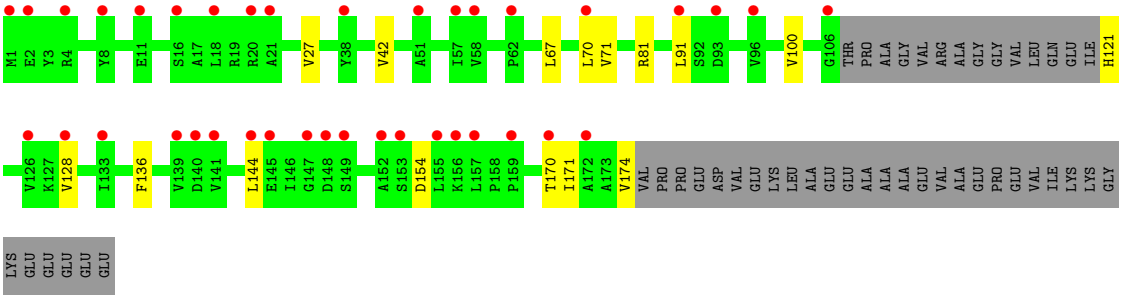
• Molecule 21: 50S ribosomal protein L25

Chain 1Z:



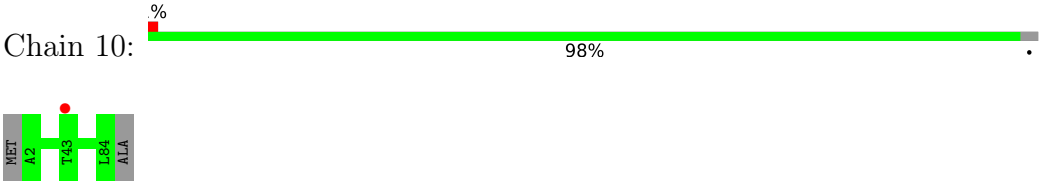
• Molecule 21: 50S ribosomal protein L25

Chain 2Z:



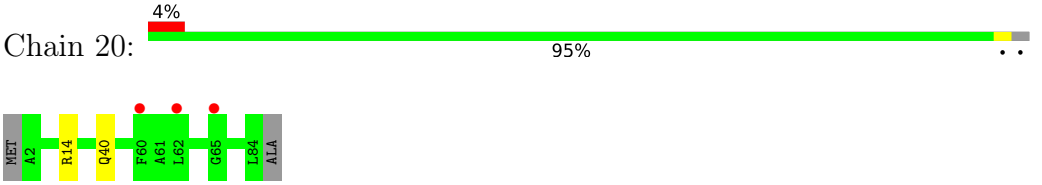
- Molecule 22: 50S ribosomal protein L27

Chain 10:



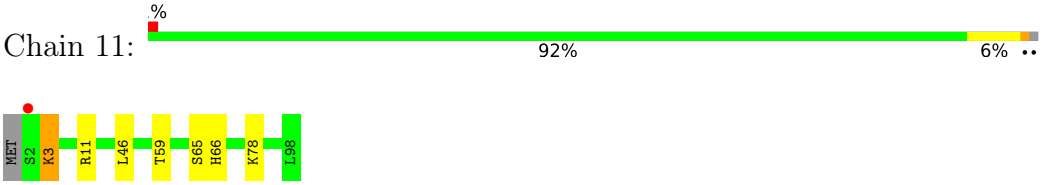
- Molecule 22: 50S ribosomal protein L27

Chain 20:



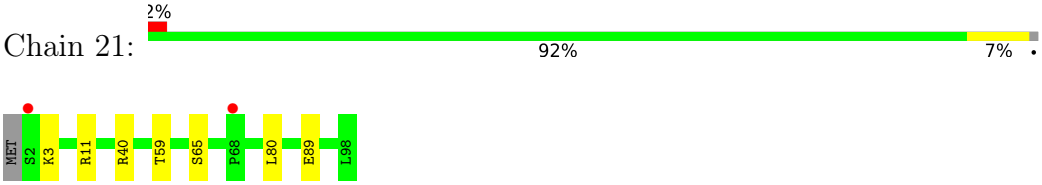
- Molecule 23: 50S ribosomal protein L28

Chain 11:



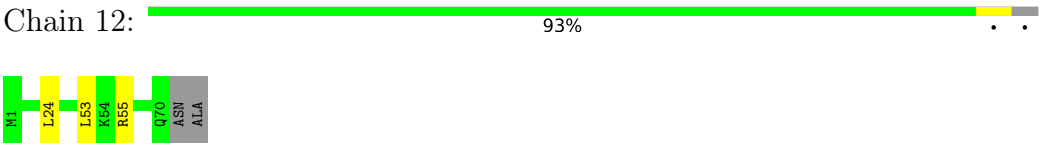
- Molecule 23: 50S ribosomal protein L28

Chain 21:



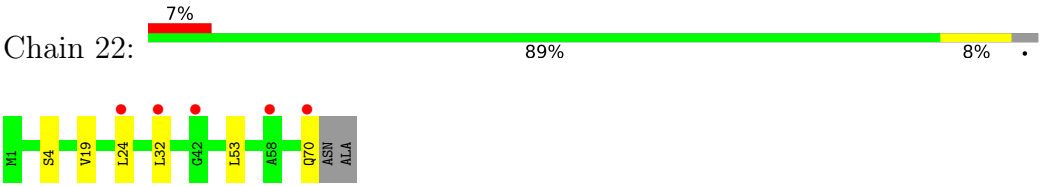
- Molecule 24: 50S ribosomal protein L29

Chain 12:



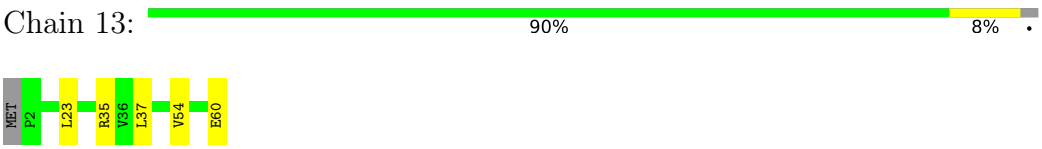
- Molecule 24: 50S ribosomal protein L29

Chain 22:



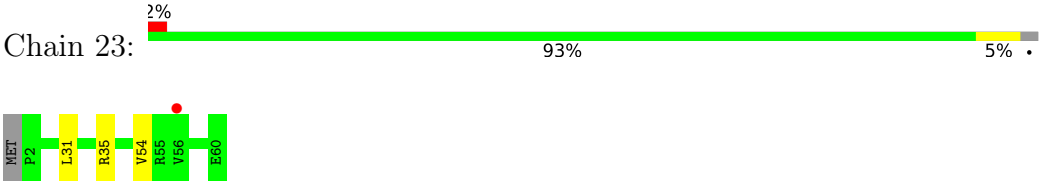
- Molecule 25: 50S ribosomal protein L30

Chain 13:



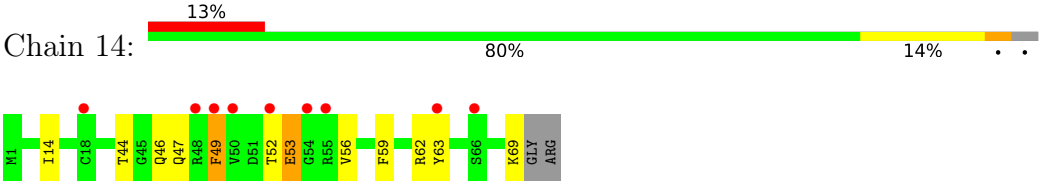
• Molecule 25: 50S ribosomal protein L30

Chain 23:



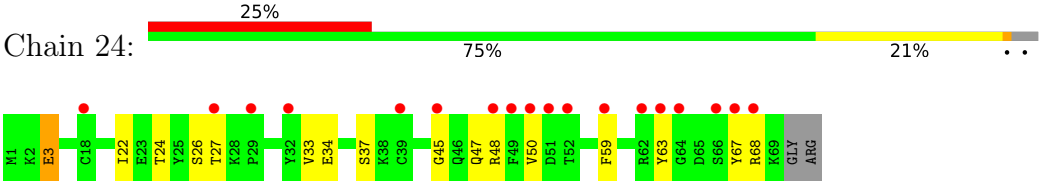
• Molecule 26: 50S ribosomal protein L31

Chain 14:



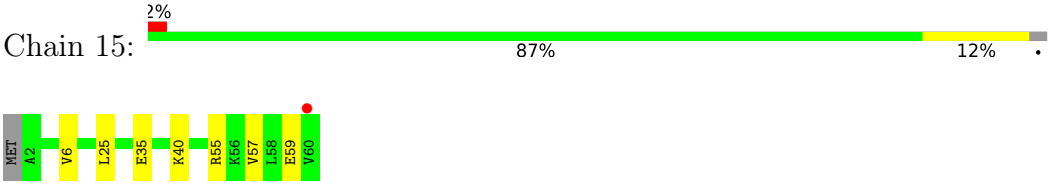
• Molecule 26: 50S ribosomal protein L31

Chain 24:



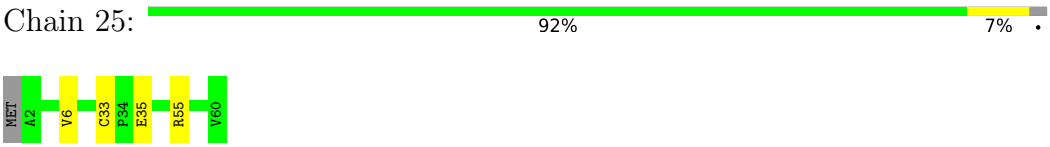
• Molecule 27: 50S ribosomal protein L32

Chain 15:



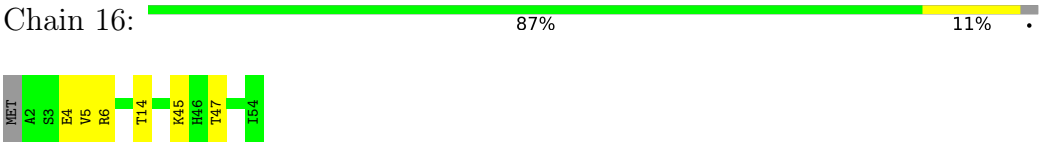
• Molecule 27: 50S ribosomal protein L32

Chain 25:



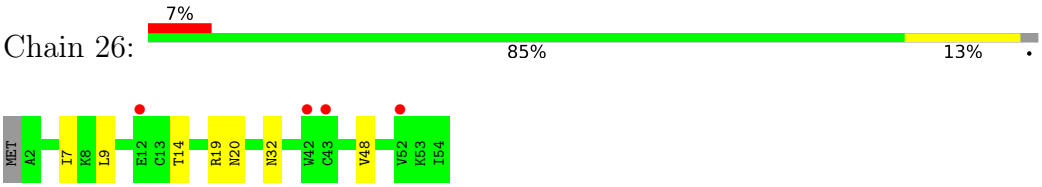
• Molecule 28: 50S ribosomal protein L33

Chain 16:



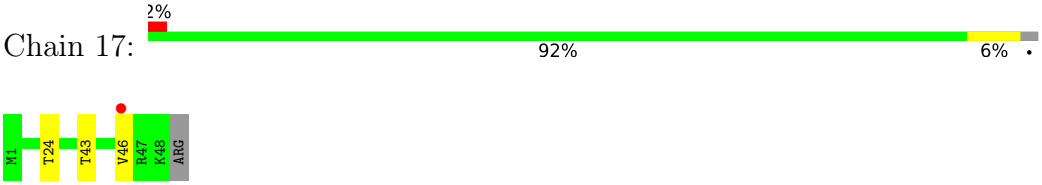
• Molecule 28: 50S ribosomal protein L33

Chain 26:



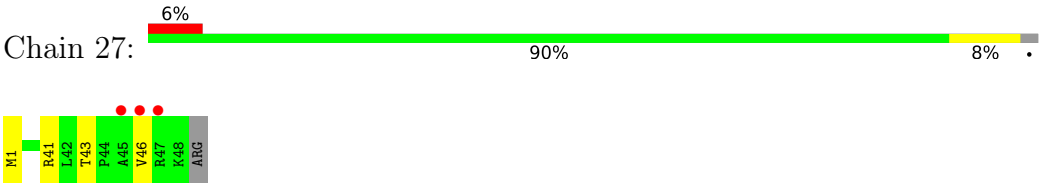
• Molecule 29: 50S ribosomal protein L34

Chain 17:



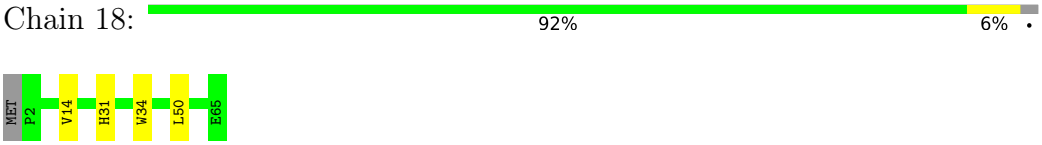
• Molecule 29: 50S ribosomal protein L34

Chain 27:



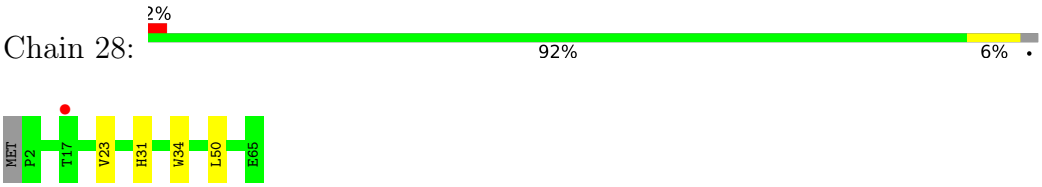
• Molecule 30: 50S ribosomal protein L35

Chain 18:



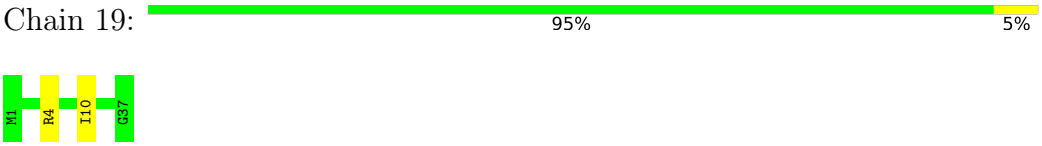
• Molecule 30: 50S ribosomal protein L35

Chain 28:



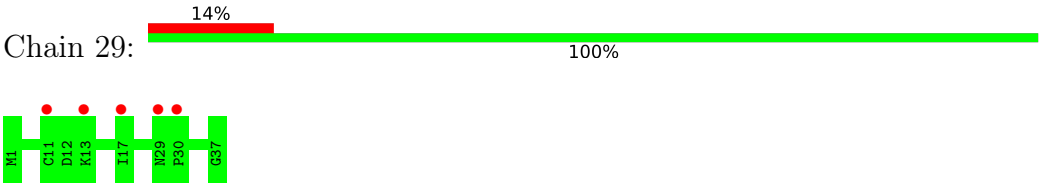
• Molecule 31: 50S ribosomal protein L36

Chain 19:



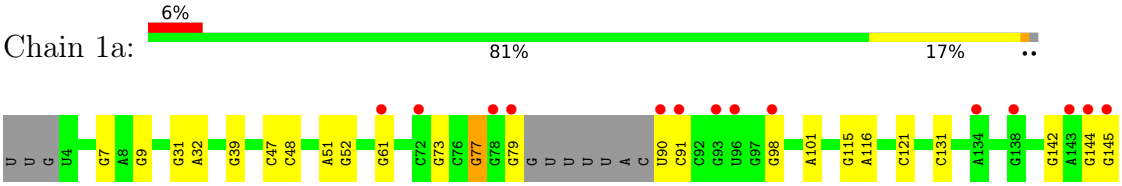
• Molecule 31: 50S ribosomal protein L36

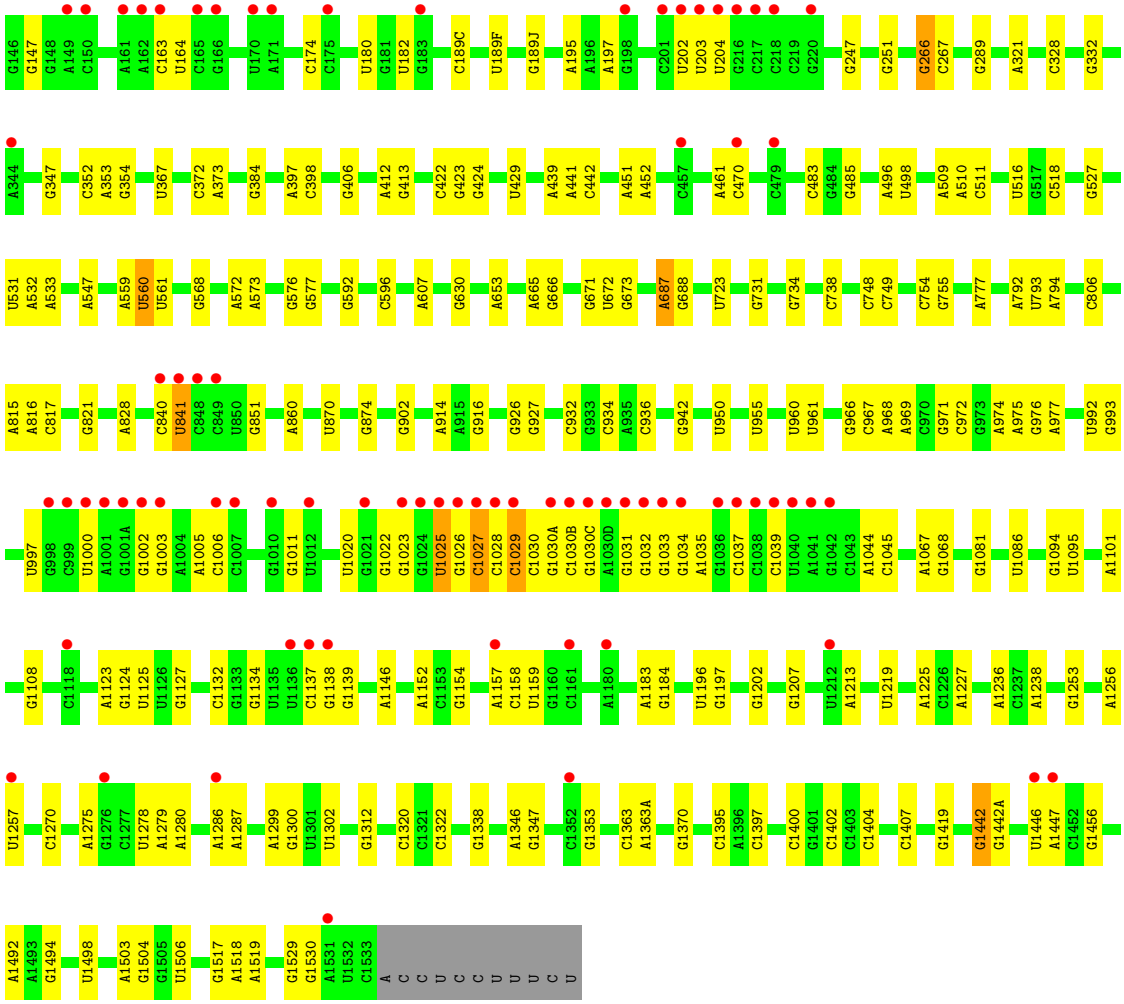
Chain 29:



• Molecule 32: 16S Ribosomal RNA

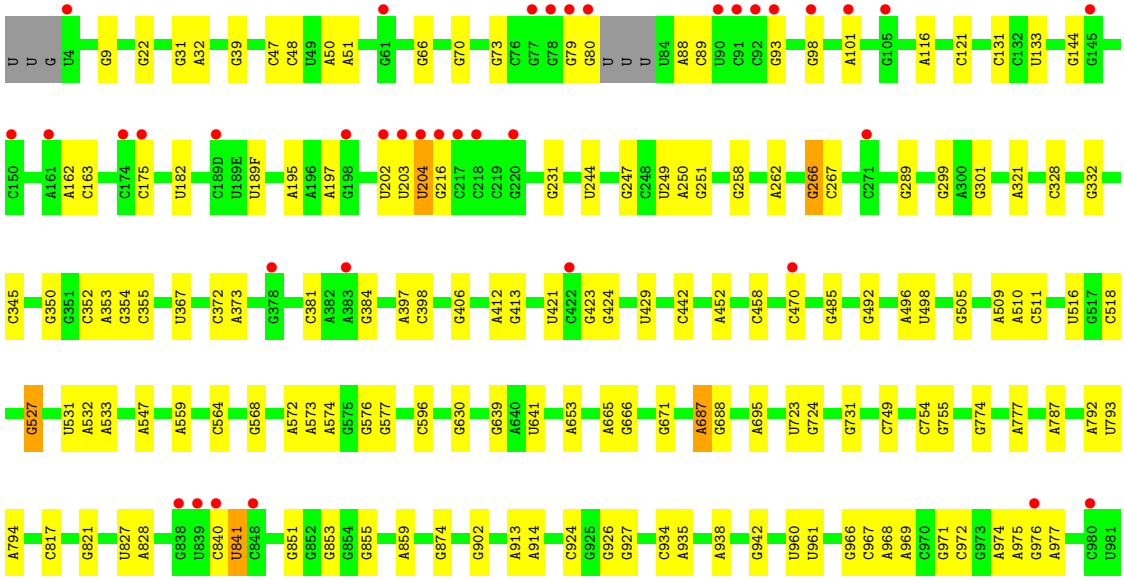
Chain 1a:

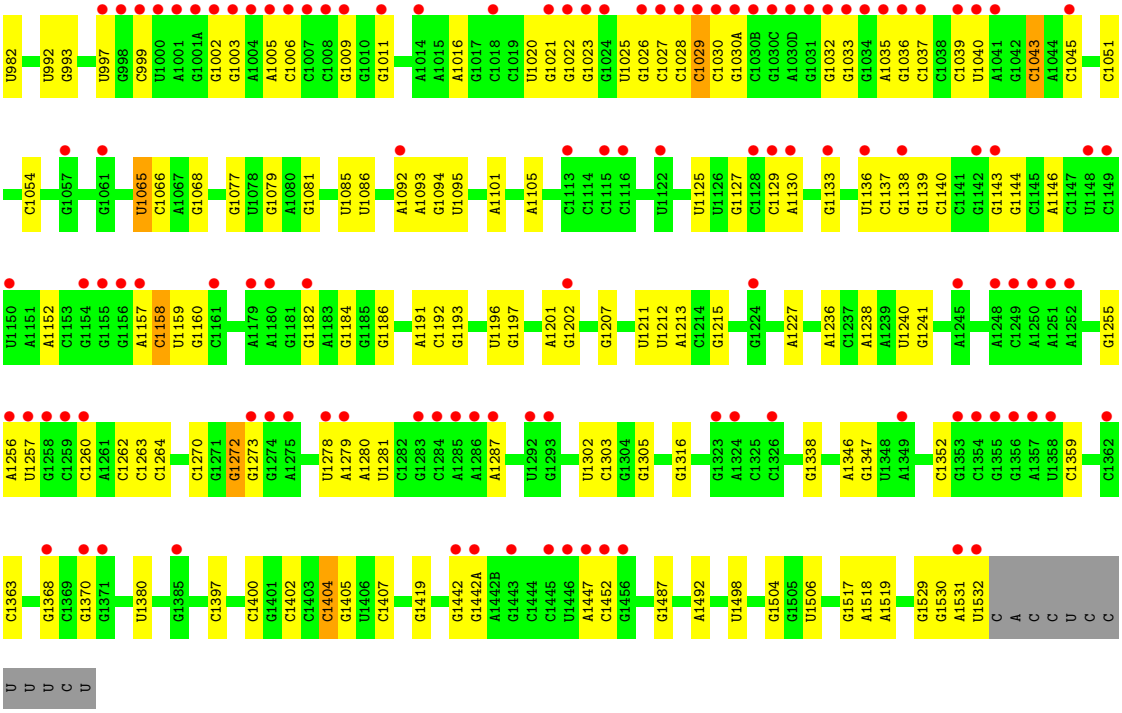




• Molecule 32: 16S Ribosomal RNA

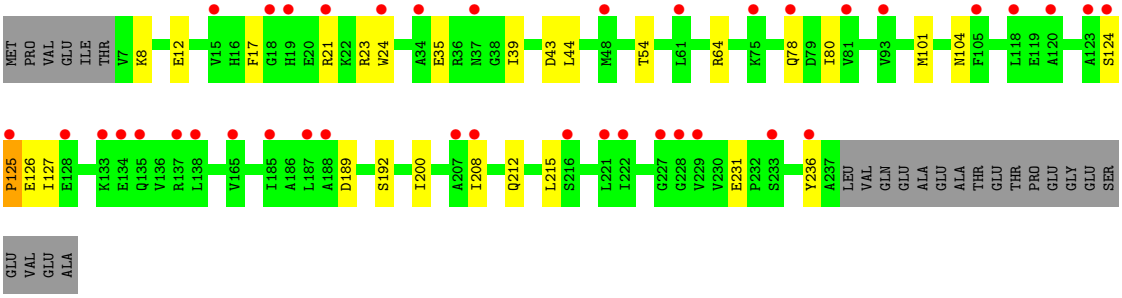
Chain 2a:





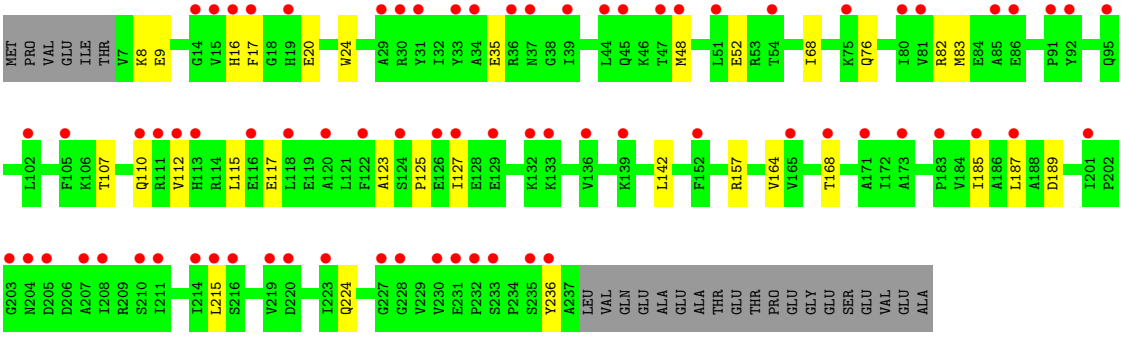
- Molecule 33: 30S ribosomal protein S2

Chain 1b:



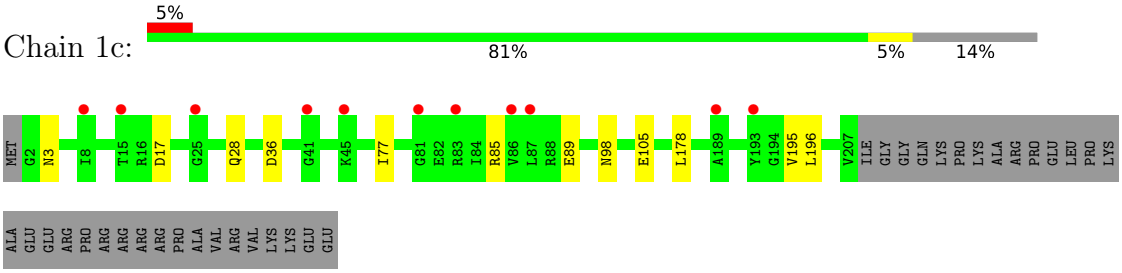
- Molecule 33: 30S ribosomal protein S2

Chain 2b:



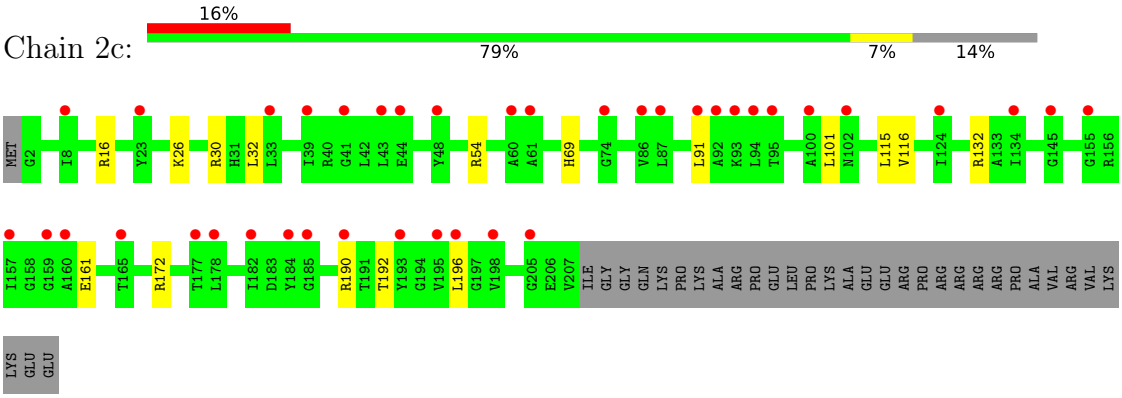
- Molecule 34: 30S ribosomal protein S3

Chain 1c:



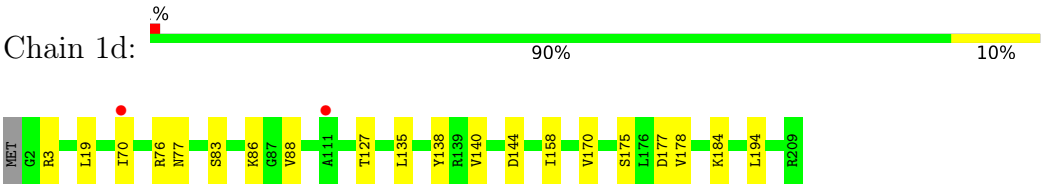
- Molecule 34: 30S ribosomal protein S3

Chain 2c:



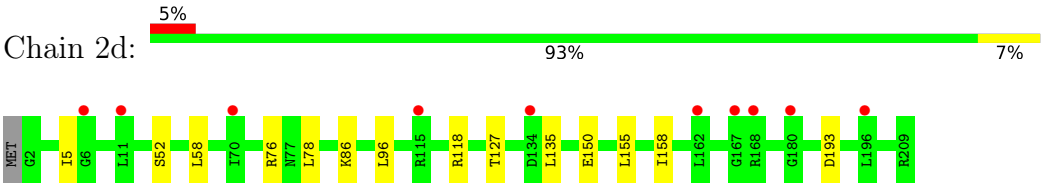
- Molecule 35: 30S ribosomal protein S4

Chain 1d:



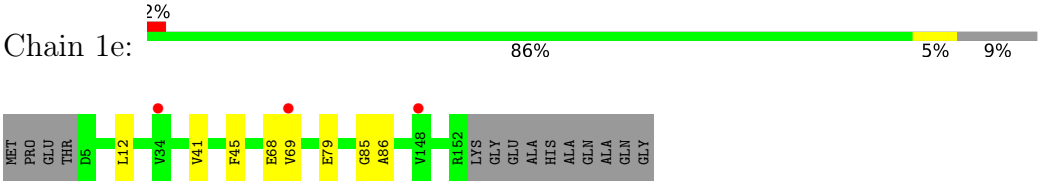
- Molecule 35: 30S ribosomal protein S4

Chain 2d:



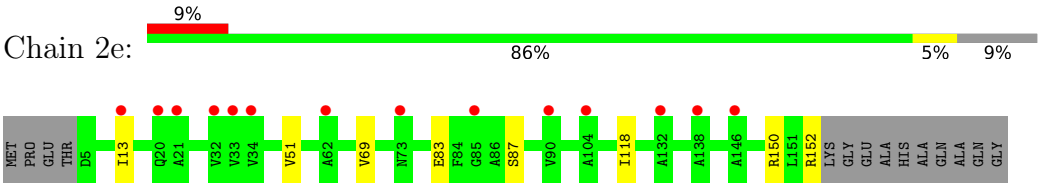
- Molecule 36: 30S ribosomal protein S5

Chain 1e:



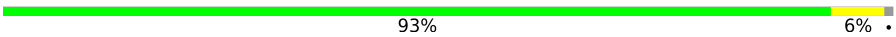
- Molecule 36: 30S ribosomal protein S5

Chain 2e:



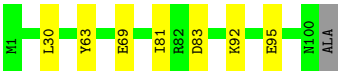
• Molecule 37: 30S ribosomal protein S6

Chain 1f:



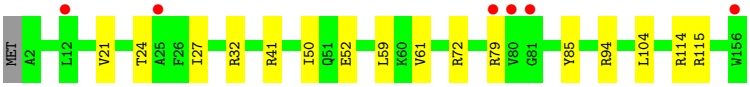
• Molecule 37: 30S ribosomal protein S6

Chain 2f:



• Molecule 38: 30S ribosomal protein S7

Chain 1g:

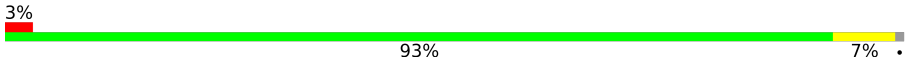


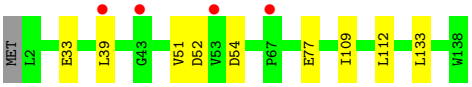
• Molecule 38: 30S ribosomal protein S7

Chain 2g:

• Molecule 39: 30S ribosomal protein S8

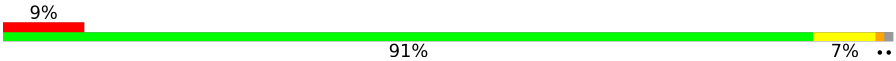
Chain 1h:

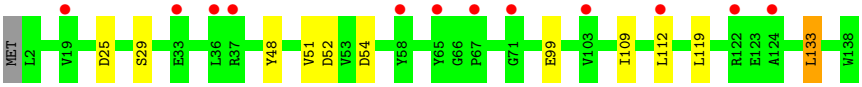




• Molecule 39: 30S ribosomal protein S8

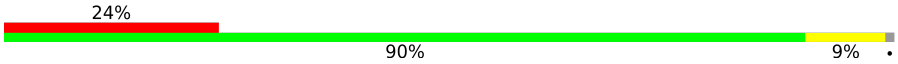
Chain 2h:

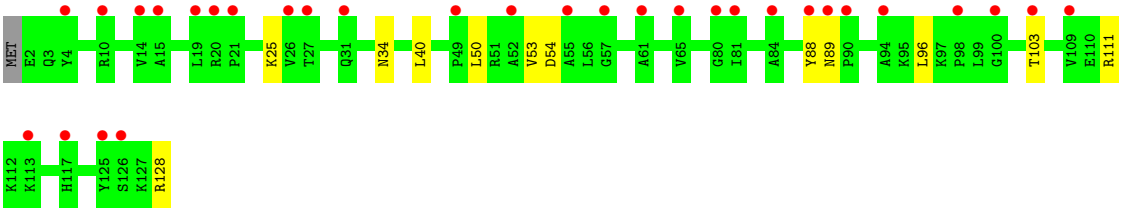




• Molecule 40: 30S ribosomal protein S9

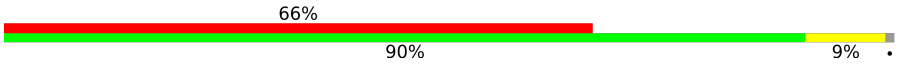
Chain 1i:

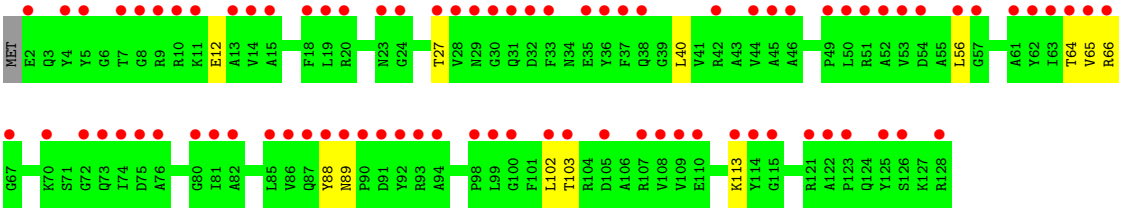




- Molecule 40: 30S ribosomal protein S9

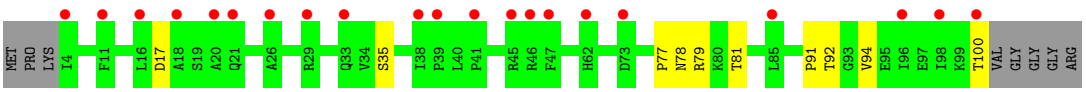
Chain 2i:





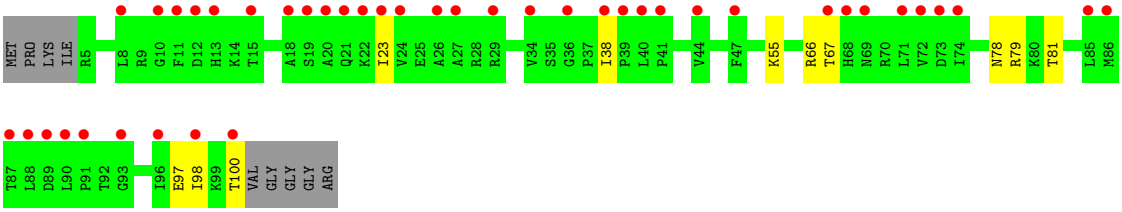
- Molecule 41: 30S ribosomal protein S10

Chain 1j:



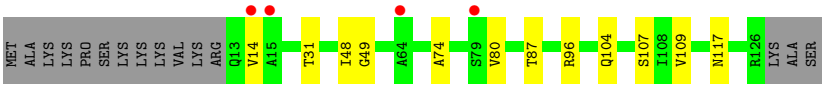
- Molecule 41: 30S ribosomal protein S10

Chain 2j:



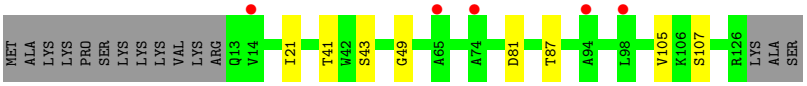
- Molecule 42: 30S ribosomal protein S11

Chain 1k:



- Molecule 42: 30S ribosomal protein S11

Chain 2k:

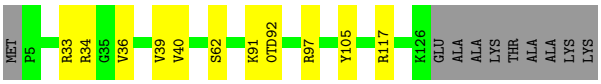


• Molecule 43: 30S ribosomal protein S12

Chain 1l:

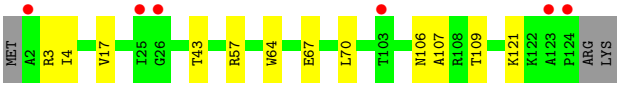
• Molecule 43: 30S ribosomal protein S12

Chain 2l:



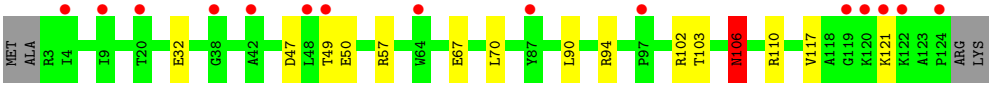
• Molecule 44: 30S ribosomal protein S13

Chain 1m:



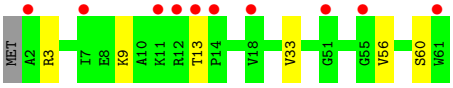
• Molecule 44: 30S ribosomal protein S13

Chain 2m:



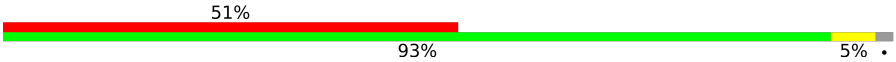
• Molecule 45: 30S ribosomal protein S14 type Z

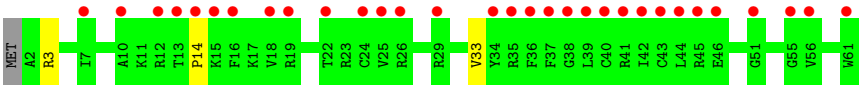
Chain 1n:



• Molecule 45: 30S ribosomal protein S14 type Z

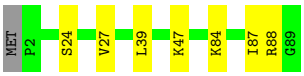
Chain 2n:





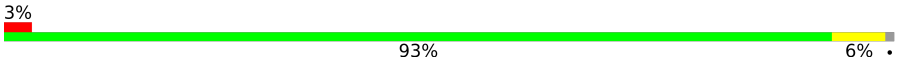
• Molecule 46: 30S ribosomal protein S15

Chain 1o:



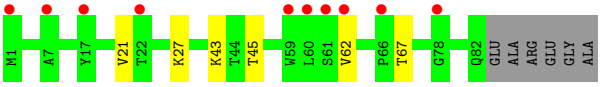
• Molecule 46: 30S ribosomal protein S15

Chain 2o:



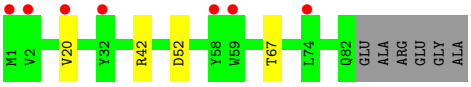
• Molecule 47: 30S ribosomal protein S16

Chain 1p:



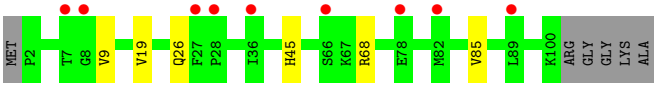
• Molecule 47: 30S ribosomal protein S16

Chain 2p:



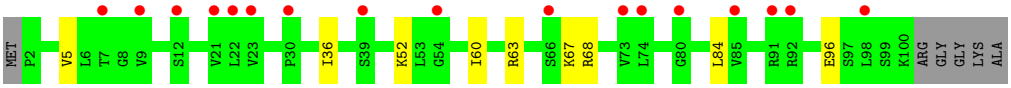
• Molecule 48: 30S ribosomal protein S17

Chain 1q:



• Molecule 48: 30S ribosomal protein S17

Chain 2q:

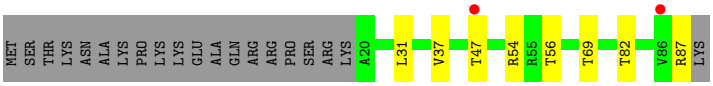


• Molecule 49: 30S ribosomal protein S18

Chain 1r:

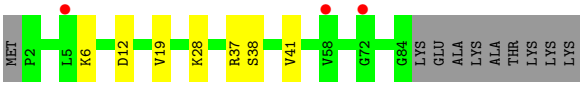
• Molecule 49: 30S ribosomal protein S18

Chain 2r:



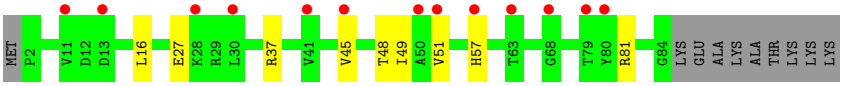
• Molecule 50: 30S ribosomal protein S19

Chain 1s:



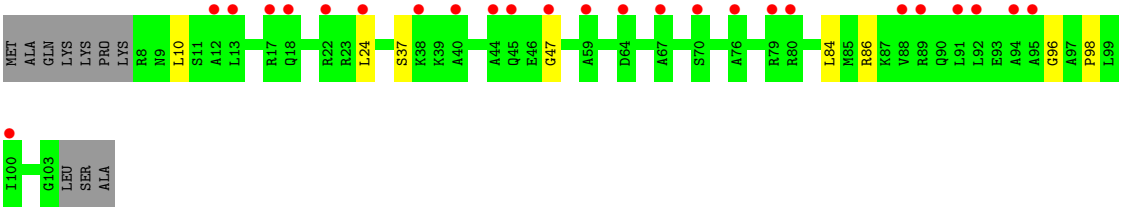
• Molecule 50: 30S ribosomal protein S19

Chain 2s:



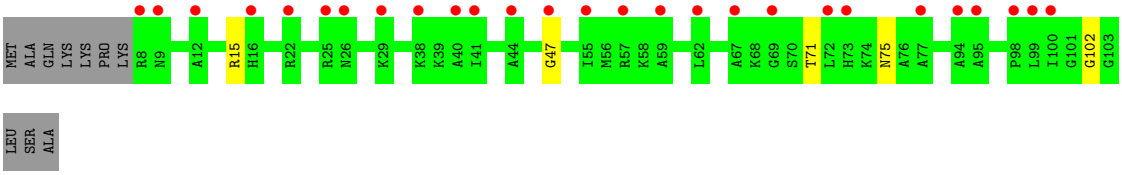
• Molecule 51: 30S ribosomal protein S20

Chain 1t:



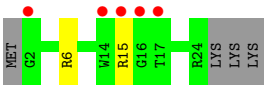
• Molecule 51: 30S ribosomal protein S20

Chain 2t:



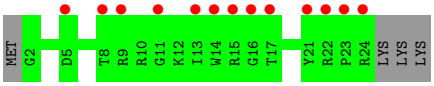
• Molecule 52: 30S ribosomal protein Thx

Chain 1u:



• Molecule 52: 30S ribosomal protein Thx

Chain 2u:

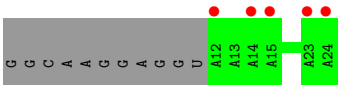


• Molecule 53: MF-mRNA

Chain 1v:

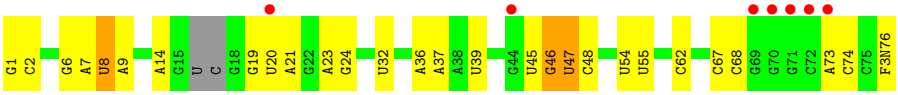
• Molecule 53: MF-mRNA

Chain 2v:



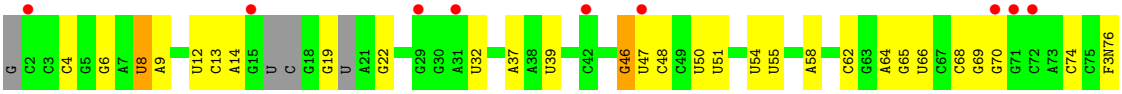
• Molecule 54: A-site Aminoacyl-tRNA Phe-NH-tRNAphe

Chain 1w:



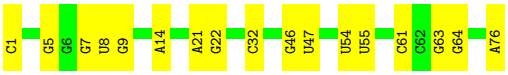
• Molecule 54: A-site Aminoacyl-tRNA Phe-NH-tRNAphe

Chain 2w:



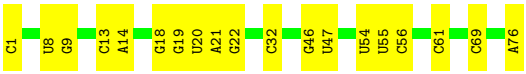
• Molecule 55: P-site Peptidyl-tRNA fMSEAC-NH-tRNAmet RNA-part

Chain 1x:



• Molecule 55: P-site Peptidyl-tRNA fMSEAC-NH-tRNAmet RNA-part

Chain 2x:



• Molecule 56: P-site Peptidyl-tRNA fMSEAC-NH-tRNAmet Peptide-part

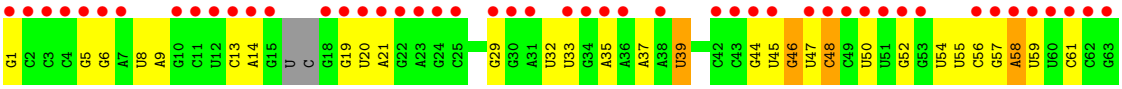
Chain 1z:

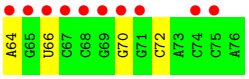
• Molecule 56: P-site Peptidyl-tRNA fMSEAC-NH-tRNAmet Peptide-part

Chain 2z:

• Molecule 57: E-site Deacylated tRNAphe

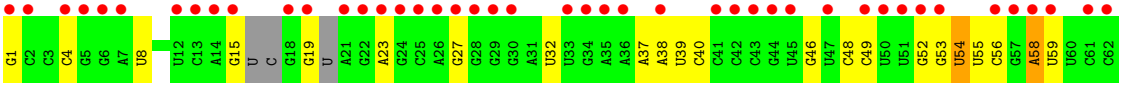
Chain 1y:

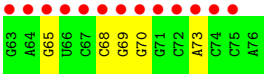




• Molecule 57: E-site Deacylated tRNAphe

Chain 2y:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	210.47Å 451.32Å 627.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	109.89 – 2.40 174.81 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.1 (109.89-2.40) 98.1 (174.81-2.40)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.23 (at 2.40Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.246 , 0.295 0.246 , 0.295	Depositor DCC
R_{free} test set	112777 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	42.3	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 50.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.34$, $< L^2 > = 0.17$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	299959	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.72% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, F3N, 2MA, ZN, PSU, 8AN, 4OC, K, 2MG, 5MC, MIA, OMC, G7M, OMG, MA6, M2G, 4SU, UR3, SF4, 5MU, OMU, 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	0/69011	1.02	81/107720 (0.1%)
1	2A	0.39	0/67295	0.90	38/105042 (0.0%)
2	1B	0.44	1/2882 (0.0%)	0.90	0/4494
2	2B	0.39	1/2879 (0.0%)	0.88	2/4487 (0.0%)
3	1D	0.35	0/2186	0.55	0/2944
3	2D	0.32	0/2186	0.52	0/2944
4	1E	0.35	0/1592	0.54	0/2149
4	2E	0.29	0/1592	0.50	0/2149
5	1F	0.34	0/1618	0.55	0/2191
5	2F	0.30	0/1614	0.50	0/2186
6	1G	0.30	0/1448	0.51	1/1957 (0.1%)
6	2G	0.28	0/1453	0.48	0/1963
7	1H	0.32	0/1356	0.49	0/1834
7	2H	0.28	0/1356	0.48	0/1834
8	1I	0.29	0/1112	0.50	0/1514
8	2I	0.29	0/1079	0.53	1/1475 (0.1%)
9	1N	0.35	0/1144	0.53	0/1543
9	2N	0.29	0/1144	0.46	0/1543
10	1O	0.34	0/943	0.53	0/1269
10	2O	0.31	0/943	0.52	0/1269
11	1P	0.32	0/1152	0.57	0/1533
11	2P	0.30	0/1152	0.54	0/1533
12	1Q	0.34	0/1143	0.53	0/1527
12	2Q	0.30	0/1143	0.50	0/1527
13	1R	0.34	0/982	0.58	0/1312
13	2R	0.28	0/982	0.50	0/1312
14	1S	0.31	0/883	0.53	0/1176
14	2S	0.29	0/880	0.48	0/1172
15	1T	0.32	0/1105	0.54	0/1477
15	2T	0.29	0/1097	0.49	0/1468
16	1U	0.34	0/977	0.54	1/1301 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	2U	0.30	0/977	0.45	0/1301
17	1V	0.34	0/782	0.59	0/1049
17	2V	0.29	0/782	0.52	0/1049
18	1W	0.35	0/897	0.57	0/1205
18	2W	0.30	0/897	0.47	0/1205
19	1X	0.36	0/764	0.57	0/1025
19	2X	0.29	0/764	0.54	0/1025
20	1Y	0.32	0/819	0.52	0/1095
20	2Y	0.31	0/819	0.49	0/1095
21	1Z	0.29	0/1267	0.52	0/1717
21	2Z	0.30	0/1299	0.51	0/1763
22	10	0.34	0/662	0.52	0/881
22	20	0.30	0/662	0.48	0/881
23	11	0.32	0/762	0.51	0/1014
23	21	0.28	0/762	0.49	0/1014
24	12	0.30	0/590	0.45	0/781
24	22	0.29	0/590	0.44	0/781
25	13	0.34	0/474	0.55	0/635
25	23	0.28	0/469	0.46	0/630
26	14	0.31	0/565	0.52	0/761
26	24	0.30	0/545	0.51	0/737
27	15	0.33	0/469	0.67	1/635 (0.2%)
27	25	0.29	0/469	0.54	0/635
28	16	0.31	0/460	0.54	0/613
28	26	0.28	0/456	0.50	0/608
29	17	0.35	0/426	0.59	0/561
29	27	0.29	0/426	0.49	0/561
30	18	0.33	0/525	0.53	0/691
30	28	0.28	0/525	0.48	0/691
31	19	0.35	0/310	0.54	0/407
31	29	0.28	0/310	0.52	0/407
32	1a	0.36	0/35795	0.90	39/55864 (0.1%)
32	2a	0.35	2/35886 (0.0%)	0.90	40/56005 (0.1%)
33	1b	0.29	0/1881	0.49	0/2542
33	2b	0.29	0/1860	0.47	0/2518
34	1c	0.29	0/1572	0.49	0/2126
34	2c	0.28	0/1566	0.48	0/2119
35	1d	0.29	0/1685	0.47	0/2262
35	2d	0.29	0/1704	0.47	0/2284
36	1e	0.29	0/1145	0.52	0/1543
36	2e	0.29	0/1149	0.49	0/1548
37	1f	0.28	0/823	0.51	0/1115
37	2f	0.29	0/829	0.51	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	1g	0.28	0/1250	0.44	0/1679
38	2g	0.28	0/1254	0.44	0/1683
39	1h	0.28	0/1108	0.46	0/1494
39	2h	0.28	0/1108	0.47	0/1494
40	1i	0.29	0/1002	0.51	0/1346
40	2i	0.30	0/997	0.50	0/1343
41	1j	0.27	0/722	0.48	0/982
41	2j	0.28	0/727	0.49	0/988
42	1k	0.28	0/844	0.48	0/1145
42	2k	0.29	0/848	0.48	0/1149
43	1l	0.31	0/937	0.53	0/1260
43	2l	0.29	0/937	0.50	0/1260
44	1m	0.28	0/969	0.53	0/1302
44	2m	0.27	0/961	0.47	0/1291
45	1n	0.31	0/501	0.48	0/664
45	2n	0.30	0/501	0.49	0/664
46	1o	0.27	0/739	0.42	0/985
46	2o	0.26	0/739	0.43	0/985
47	1p	0.26	0/697	0.50	0/939
47	2p	0.27	0/693	0.50	0/935
48	1q	0.29	0/836	0.48	0/1117
48	2q	0.29	0/836	0.47	0/1117
49	1r	0.28	0/560	0.49	0/746
49	2r	0.28	0/560	0.48	0/746
50	1s	0.29	0/667	0.53	0/900
50	2s	0.30	0/661	0.57	0/893
51	1t	0.27	0/730	0.46	0/965
51	2t	0.27	0/729	0.42	0/965
52	1u	0.27	0/203	0.49	0/266
52	2u	0.27	0/203	0.51	0/266
53	1v	0.39	0/310	0.87	0/480
53	2v	0.38	0/310	0.82	0/480
54	1w	0.54	1/1581 (0.1%)	1.10	2/2458 (0.1%)
54	2w	0.43	0/1531	1.06	0/2379
55	1x	0.61	2/1723 (0.1%)	1.16	22/2684 (0.8%)
55	2x	0.53	1/1723 (0.1%)	1.09	13/2684 (0.5%)
56	1z	0.56	0/25	0.72	0/32
56	2z	0.22	0/19	0.46	0/24
57	1y	0.57	1/1606 (0.1%)	1.16	9/2497 (0.4%)
57	2y	0.55	1/1583 (0.1%)	1.09	3/2459 (0.1%)
All	All	0.39	10/316678 (0.0%)	0.85	253/474093 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

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

Mol	Chain	#Chirality outliers	#Planarity outliers
33	1b	0	1
44	2m	0	1
All	All	0	2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	1x	1	C	OP3-P	-10.49	1.48	1.61
54	1w	1	G	OP3-P	-10.45	1.48	1.61
2	2B	1	U	OP3-P	-10.39	1.48	1.61
57	1y	1	G	OP3-P	-10.29	1.48	1.61
2	1B	1	U	OP3-P	-10.22	1.48	1.61
55	2x	1	C	OP3-P	-10.21	1.48	1.61
57	2y	1	G	OP3-P	-10.19	1.49	1.61
32	2a	1272	G	N1-C2	-7.40	1.31	1.37
32	2a	1272	G	C6-N1	-6.96	1.34	1.39
55	1x	22	G	N7-C5	6.59	1.43	1.39

All (253) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	1263	C	N1-C2-O2	20.49	131.19	118.90
32	2a	1272	G	N3-C2-N2	18.78	133.05	119.90
32	2a	1272	G	N1-C2-N2	-15.88	101.91	116.20
32	2a	1272	G	C5-C6-O6	15.62	137.97	128.60
32	2a	1263	C	C2-N3-C4	13.48	126.64	119.90
32	2a	1272	G	C6-N1-C2	11.86	132.22	125.10
1	1A	1086	A	N1-C6-N6	-11.56	111.66	118.60
32	2a	1272	G	C5-C6-N1	-10.95	106.03	111.50
32	2a	1263	C	C5-C6-N1	10.84	126.42	121.00
55	1x	46	G	C6-N1-C2	-10.76	118.64	125.10
1	1A	1075	C	N1-C2-O2	10.20	125.02	118.90
32	2a	1263	C	N3-C2-O2	-10.13	114.81	121.90
1	1A	999	U	O5'-P-OP2	-9.87	96.81	105.70
1	1A	1063	G	C5-C6-O6	9.81	134.49	128.60
55	2x	46	G	C6-N1-C2	-9.77	119.24	125.10
55	2x	14	A	C4-C5-C6	9.66	121.83	117.00
55	1x	14	A	C4-C5-C6	9.47	121.74	117.00
1	1A	1075	C	C2-N3-C4	9.29	124.54	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	1x	14	A	C5-N7-C8	9.19	108.50	103.90
1	1A	2577	A	O5'-P-OP1	-9.17	97.44	105.70
55	1x	22	G	N1-C6-O6	-8.61	114.73	119.90
55	1x	22	G	C4-C5-C6	-8.48	113.71	118.80
1	1A	512	G	O4'-C1'-N9	8.22	114.77	108.20
32	2a	1263	C	C4-C5-C6	-8.16	113.32	117.40
32	2a	754	C	N1-C2-O2	8.16	123.80	118.90
1	1A	2167	U	C2-N1-C1'	8.14	127.47	117.70
55	1x	14	A	C5-C6-N1	-8.03	113.69	117.70
32	2a	754	C	C2-N1-C1'	7.99	127.59	118.80
1	1A	567	A	O5'-P-OP1	-7.99	98.51	105.70
55	1x	22	G	C5-N7-C8	-7.98	100.31	104.30
32	2a	1272	G	C2-N3-C4	-7.89	107.95	111.90
32	1a	1030(B)	C	N1-C2-O2	7.59	123.45	118.90
1	1A	1063	G	C6-N1-C2	7.57	129.64	125.10
32	2a	1263	C	N1-C2-N3	-7.48	113.97	119.20
1	1A	2554	U	O5'-P-OP1	-7.43	99.01	105.70
32	1a	1158	C	C2-N1-C1'	7.38	126.91	118.80
55	2x	14	A	C5-N7-C8	7.34	107.57	103.90
32	2a	1263	C	C2-N1-C1'	7.32	126.85	118.80
1	2A	1313	U	C2-N1-C1'	7.29	126.45	117.70
32	1a	1030(B)	C	C2-N1-C1'	7.28	126.81	118.80
1	1A	1063	G	N3-C2-N2	7.18	124.92	119.90
1	1A	2167	U	N1-C2-O2	7.13	127.79	122.80
32	2a	1272	G	C4-N9-C1'	7.13	135.78	126.50
57	1y	33	U	N1-C2-O2	7.07	127.75	122.80
1	1A	2682	U	O5'-P-OP2	-7.05	99.35	105.70
1	1A	2492	U	O5'-P-OP1	-7.05	99.36	105.70
32	2a	1272	G	C8-N9-C1'	-7.01	117.89	127.00
1	2A	2129	C	N1-C2-O2	6.99	123.10	118.90
32	2a	1043	C	N1-C2-O2	6.98	123.09	118.90
32	2a	1158	C	C2-N1-C1'	6.95	126.45	118.80
55	2x	22	G	C5-N7-C8	-6.95	100.83	104.30
32	1a	1034	G	C5-C6-O6	6.94	132.76	128.60
32	2a	1054	C	C2-N1-C1'	6.92	126.42	118.80
57	1y	33	U	C2-N1-C1'	6.91	125.99	117.70
1	1A	1352	U	O5'-P-OP1	-6.90	99.49	105.70
32	1a	1029	C	C2-N3-C4	6.89	123.34	119.90
32	1a	1158	C	N1-C2-O2	6.89	123.03	118.90
32	2a	754	C	N3-C2-O2	-6.86	117.10	121.90
32	1a	266	G	P-O3'-C3'	6.86	127.93	119.70
1	2A	2136	C	N1-C2-O2	6.82	122.99	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	2714	G	O5'-P-OP2	-6.80	99.58	105.70
55	1x	22	G	N3-C4-N9	-6.80	121.92	126.00
32	1a	841	U	C5-C6-N1	6.77	126.08	122.70
1	1A	996	A	O5'-P-OP1	-6.76	99.62	105.70
1	1A	748	G	O4'-C1'-N9	6.75	113.60	108.20
55	2x	14	A	C5-C6-N1	-6.70	114.35	117.70
1	1A	1187	G	N1-C6-O6	-6.69	115.89	119.90
54	1w	47	U	C2-N1-C1'	6.65	125.68	117.70
1	2A	2689	U	P-O3'-C3'	6.58	127.59	119.70
1	2A	2159	G	N3-C2-N2	6.56	124.49	119.90
1	1A	1992	G	P-O3'-C3'	6.54	127.55	119.70
32	2a	1262	C	N1-C2-O2	6.54	122.83	118.90
32	2a	1272	G	N1-C6-O6	-6.54	115.97	119.90
57	1y	50	U	C5-C4-O4	6.52	129.81	125.90
1	2A	2155	G	C6-N1-C2	6.48	128.99	125.10
57	1y	64	A	C5-C6-N6	6.48	128.88	123.70
2	2B	1	U	C2-N1-C1'	6.46	125.46	117.70
32	1a	754	C	C2-N1-C1'	6.46	125.91	118.80
57	1y	33	U	N3-C2-O2	-6.40	117.72	122.20
55	1x	46	G	N1-C2-N3	6.38	127.73	123.90
1	2A	1698	A	O4'-C1'-N9	6.37	113.30	108.20
1	1A	975	C	N1-C2-O2	-6.37	115.08	118.90
32	1a	90	U	N3-C2-O2	-6.37	117.74	122.20
32	1a	1034	G	C6-N1-C2	6.37	128.92	125.10
55	1x	22	G	C6-C5-N7	6.36	134.21	130.40
1	2A	2159	G	C6-N1-C2	6.35	128.91	125.10
1	1A	2608	G	C5-C6-O6	-6.34	124.80	128.60
1	1A	2167	U	N3-C2-O2	-6.30	117.79	122.20
1	1A	787	U	O5'-P-OP1	-6.30	100.03	105.70
1	1A	226	G	O4'-C1'-N9	6.26	113.20	108.20
1	1A	1063	G	N1-C6-O6	-6.25	116.15	119.90
32	1a	1025	U	N1-C2-O2	6.24	127.17	122.80
32	1a	1030(B)	C	C6-N1-C2	-6.24	117.80	120.30
1	1A	963	U	O5'-P-OP2	-6.22	100.10	105.70
1	1A	2608	G	N1-C6-O6	6.21	123.62	119.90
1	1A	847	U	C2-N1-C1'	6.18	125.12	117.70
1	1A	576	U	O5'-P-OP1	-6.15	100.17	105.70
55	1x	46	G	N9-C4-C5	6.14	107.86	105.40
57	1y	50	U	C2-N3-C4	6.12	130.67	127.00
27	15	25	LEU	C-N-CA	-6.11	106.42	121.70
1	2A	1639	U	O5'-P-OP2	-6.10	100.21	105.70
1	2A	192	C	O5'-P-OP1	-6.08	100.23	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1263	C	C6-N1-C2	-6.07	117.87	120.30
32	1a	560	U	C2-N1-C1'	6.04	124.94	117.70
1	1A	1993	U	O5'-P-OP1	-6.01	100.29	105.70
1	1A	746	A	O4'-C1'-N9	6.01	113.00	108.20
1	1A	1086	A	C5-C6-N6	6.00	128.50	123.70
1	1A	2629	A	P-O3'-C3'	5.99	126.89	119.70
1	2A	752	A	P-O3'-C3'	5.99	126.88	119.70
32	1a	90	U	C2-N1-C1'	5.95	124.84	117.70
2	2B	80	U	O4'-C1'-N1	5.95	112.96	108.20
57	1y	48	C	N1-C2-O2	-5.95	115.33	118.90
1	1A	2848	G	O4'-C1'-N9	5.95	112.96	108.20
1	1A	1082	U	N3-C4-O4	-5.93	115.25	119.40
1	1A	1187	G	C5-C6-O6	5.93	132.16	128.60
32	1a	754	C	C6-N1-C2	-5.91	117.94	120.30
32	2a	841	U	C5-C6-N1	5.89	125.64	122.70
32	1a	841	U	C2-N1-C1'	5.88	124.75	117.70
55	1x	22	G	C8-N9-C1'	5.87	134.63	127.00
1	2A	2155	G	C5-C6-O6	5.86	132.12	128.60
57	2y	58	A	C4-C5-C6	5.84	119.92	117.00
1	1A	1188	U	N1-C2-O2	5.80	126.86	122.80
1	1A	1074	G	N9-C4-C5	-5.80	103.08	105.40
1	1A	2587	A	OP1-P-O3'	5.79	117.93	105.20
1	1A	1992	G	C8-N9-C4	-5.78	104.09	106.40
1	2A	90	U	N3-C2-O2	-5.78	118.16	122.20
1	1A	250	G	C8-N9-C4	-5.77	104.09	106.40
32	1a	1395	C	C2-N3-C4	5.77	122.78	119.90
1	2A	512	G	O4'-C1'-N9	5.76	112.81	108.20
32	1a	1030(B)	C	N3-C2-O2	-5.76	117.87	121.90
55	1x	22	G	C5-C6-N1	5.75	114.38	111.50
55	1x	46	G	N3-C2-N2	-5.75	115.88	119.90
1	1A	1905	C	N1-C2-O2	5.74	122.34	118.90
1	2A	746	A	O4'-C1'-N9	5.71	112.77	108.20
57	2y	58	A	N1-C6-N6	5.71	122.03	118.60
55	2x	14	A	C8-N9-C1'	-5.70	117.44	127.70
1	2A	2129	C	C2-N3-C4	5.69	122.74	119.90
32	2a	1158	C	N1-C2-O2	5.68	122.31	118.90
1	1A	1075	C	C5-C4-N4	5.67	124.17	120.20
1	1A	2067	G	C8-N9-C4	-5.67	104.13	106.40
32	2a	1263	C	C5-C4-N4	5.67	124.17	120.20
1	2A	1313	U	N1-C2-O2	5.66	126.76	122.80
32	2a	299	G	C5-C6-O6	-5.66	125.20	128.60
55	1x	46	G	C5-C6-N1	5.65	114.33	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	2I	77	LEU	CA-CB-CG	5.65	128.29	115.30
32	1a	1442	G	N3-C4-C5	-5.64	125.78	128.60
1	2A	9	U	C5-C6-N1	5.64	125.52	122.70
1	1A	1075	C	N3-C2-O2	-5.63	117.96	121.90
32	1a	1032	G	C6-N1-C2	5.62	128.47	125.10
1	2A	1313	U	N3-C2-O2	-5.62	118.26	122.20
1	2A	1614	A	O5'-P-OP1	-5.61	100.65	105.70
32	2a	754	C	C6-N1-C1'	-5.61	114.07	120.80
1	1A	1174	A	P-O3'-C3'	5.60	126.42	119.70
55	2x	46	G	C5-C6-N1	5.59	114.30	111.50
55	2x	22	G	C4-C5-C6	-5.59	115.44	118.80
1	1A	1064	C	C5-C6-N1	5.59	123.79	121.00
55	2x	14	A	N1-C6-N6	5.58	121.95	118.60
1	1A	1905	C	C2-N1-C1'	5.57	124.93	118.80
55	2x	14	A	C4-N9-C1'	5.57	136.32	126.30
1	1A	2790	A	C2-N3-C4	5.56	113.38	110.60
32	1a	90	U	N1-C2-O2	5.56	126.69	122.80
1	1A	1064	C	N3-C4-N4	5.55	121.89	118.00
55	1x	46	G	C4-C5-N7	-5.55	108.58	110.80
1	2A	847	U	C2-N1-C1'	5.54	124.35	117.70
32	1a	77	G	C4-N9-C1'	-5.54	119.31	126.50
55	1x	46	G	C5-C6-O6	-5.54	125.28	128.60
1	1A	1082	U	N3-C4-C5	5.53	117.92	114.60
1	1A	1074	G	C4-C5-N7	5.53	113.01	110.80
1	1A	1936	A	O4'-C1'-N9	5.52	112.62	108.20
55	1x	14	A	C4-C5-N7	-5.52	107.94	110.70
32	2a	1043	C	C2-N3-C4	5.50	122.65	119.90
1	1A	1064	C	C2-N1-C1'	5.49	124.84	118.80
1	2A	2897	U	C2-N1-C1'	5.49	124.29	117.70
54	1w	47	U	N1-C2-O2	5.48	126.64	122.80
55	1x	22	G	N3-C4-C5	5.48	131.34	128.60
1	1A	2872	G	N1-C6-O6	-5.47	116.62	119.90
1	1A	1251	C	C6-N1-C2	-5.46	118.12	120.30
32	1a	1032	G	C5-C6-O6	5.46	131.88	128.60
32	1a	1067	A	P-O3'-C3'	5.46	126.25	119.70
1	1A	1614	A	O5'-P-OP1	-5.46	100.79	105.70
1	2A	898	C	C6-N1-C2	-5.45	118.12	120.30
32	1a	115	G	P-O3'-C3'	5.45	126.23	119.70
1	1A	2134	A	P-O3'-C3'	5.43	126.21	119.70
32	2a	1263	C	N3-C4-N4	-5.43	114.20	118.00
1	1A	2691	C	N1-C2-O2	5.42	122.16	118.90
1	1A	2167	U	C5-C6-N1	5.42	125.41	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	687	A	P-O3'-C3'	5.42	126.20	119.70
1	1A	444	C	O5'-P-OP1	5.41	117.19	110.70
55	2x	46	G	N3-C2-N2	-5.41	116.11	119.90
32	1a	754	C	N1-C2-O2	5.41	122.14	118.90
1	1A	2784	C	N1-C2-O2	5.40	122.14	118.90
32	2a	204	U	N1-C2-O2	5.40	126.58	122.80
1	2A	228	A	P-O3'-C3'	5.38	126.15	119.70
32	1a	1158	C	C6-N1-C1'	-5.37	114.35	120.80
32	1a	1030(B)	C	C5-C6-N1	5.37	123.68	121.00
32	2a	1158	C	C6-N1-C2	-5.36	118.16	120.30
32	1a	1029	C	N1-C2-O2	5.35	122.11	118.90
1	2A	2866	U	C2-N1-C1'	5.34	124.11	117.70
1	2A	2318	G	C4-N9-C1'	5.33	133.42	126.50
57	1y	64	A	C6-N1-C2	5.32	121.79	118.60
32	2a	266	G	N3-C4-C5	-5.31	125.94	128.60
1	2A	528	A	P-O3'-C3'	5.30	126.06	119.70
32	1a	841	U	C6-N1-C2	-5.30	117.82	121.00
1	2A	1992	G	P-O3'-C3'	5.30	126.06	119.70
1	1A	463	G	N3-C2-N2	-5.29	116.20	119.90
1	1A	1153	C	O5'-P-OP2	-5.28	100.95	105.70
32	2a	1065	U	P-O3'-C3'	5.28	126.03	119.70
1	1A	573	G	OP1-P-O3'	5.27	116.80	105.20
1	2A	2685	G	N1-C6-O6	-5.27	116.74	119.90
1	2A	2689	U	N3-C2-O2	-5.26	118.52	122.20
1	1A	2167	U	C6-N1-C1'	-5.24	113.87	121.20
32	2a	266	G	P-O3'-C3'	5.23	125.97	119.70
32	2a	1054	C	C6-N1-C1'	-5.22	114.53	120.80
32	1a	1225	A	C5-C6-N6	5.22	127.88	123.70
1	2A	801	G	O5'-P-OP2	-5.22	101.00	105.70
55	1x	14	A	C8-N9-C1'	-5.22	118.31	127.70
16	1U	74	LEU	CA-CB-CG	5.21	127.28	115.30
1	1A	2128	C	N1-C2-O2	5.20	122.02	118.90
32	1a	560	U	C3'-C2'-C1'	5.19	105.66	101.50
1	2A	265	A	O4'-C1'-N9	5.19	112.35	108.20
1	2A	748	G	O4'-C1'-N9	5.19	112.35	108.20
32	2a	913	A	P-O3'-C3'	5.18	125.92	119.70
55	2x	46	G	N1-C2-N3	5.18	127.01	123.90
1	1A	2033	A	O4'-C1'-N9	5.17	112.34	108.20
1	1A	784	A	P-O3'-C3'	5.17	125.90	119.70
1	1A	1253	A	C5-N7-C8	5.16	106.48	103.90
32	1a	687	A	P-O3'-C3'	5.16	125.90	119.70
32	1a	754	C	N3-C2-O2	-5.16	118.28	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	1325	G	N9-C4-C5	5.16	107.46	105.40
1	1A	2140	C	C2-N3-C4	5.16	122.48	119.90
1	1A	845	G	O4'-C1'-N9	5.14	112.32	108.20
32	2a	1029	C	N1-C2-O2	5.13	121.98	118.90
1	1A	1192	G	N7-C8-N9	-5.13	110.53	113.10
57	1y	58	A	P-O3'-C3'	5.12	125.85	119.70
1	2A	2155	G	N3-C2-N2	5.12	123.48	119.90
1	1A	645	C	N1-C2-O2	5.11	121.96	118.90
1	1A	1080	C	N1-C2-O2	5.10	121.96	118.90
1	1A	847	U	N1-C2-O2	5.09	126.36	122.80
1	2A	2804	C	C6-N1-C2	-5.08	118.27	120.30
32	1a	955	U	C2-N3-C4	5.07	130.04	127.00
55	1x	14	A	C4-N9-C1'	5.06	135.41	126.30
1	1A	1565	C	N1-C2-O2	5.06	121.94	118.90
57	2y	4	C	C2-N3-C4	5.06	122.43	119.90
1	2A	528	A	OP1-P-O3'	5.05	116.31	105.20
1	2A	2137	C	C6-N1-C2	-5.05	118.28	120.30
55	2x	46	G	N3-C4-C5	-5.04	126.08	128.60
55	1x	22	G	C4-N9-C1'	-5.04	119.95	126.50
32	1a	1002	G	C4-N9-C1'	5.03	133.03	126.50
6	1G	140	ILE	C-N-CA	5.02	134.25	121.70
1	2A	897	C	C5-C6-N1	5.02	123.51	121.00
32	1a	1027	C	C6-N1-C1'	5.01	126.82	120.80
32	1a	748	C	P-O3'-C3'	5.01	125.71	119.70
1	1A	1188	U	N3-C2-O2	-5.00	118.70	122.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
33	1b	125	PRO	Peptide
44	2m	106	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%)	255 (93%)	18 (7%)	0	100	100
3	2D	273/276 (99%)	255 (93%)	18 (7%)	0	100	100
4	1E	202/206 (98%)	190 (94%)	10 (5%)	2 (1%)	15	23
4	2E	202/206 (98%)	188 (93%)	13 (6%)	1 (0%)	29	41
5	1F	200/210 (95%)	194 (97%)	5 (2%)	1 (0%)	29	41
5	2F	200/210 (95%)	178 (89%)	18 (9%)	4 (2%)	7	9
6	1G	179/182 (98%)	162 (90%)	16 (9%)	1 (1%)	25	36
6	2G	179/182 (98%)	155 (87%)	19 (11%)	5 (3%)	5	4
7	1H	172/180 (96%)	160 (93%)	11 (6%)	1 (1%)	25	36
7	2H	172/180 (96%)	155 (90%)	15 (9%)	2 (1%)	13	19
8	1I	144/148 (97%)	126 (88%)	17 (12%)	1 (1%)	22	32
8	2I	144/148 (97%)	121 (84%)	22 (15%)	1 (1%)	22	32
9	1N	138/140 (99%)	135 (98%)	2 (1%)	1 (1%)	22	32
9	2N	138/140 (99%)	129 (94%)	8 (6%)	1 (1%)	22	32
10	1O	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
10	2O	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
11	1P	147/150 (98%)	129 (88%)	15 (10%)	3 (2%)	7	9
11	2P	147/150 (98%)	129 (88%)	12 (8%)	6 (4%)	3	2
12	1Q	139/141 (99%)	131 (94%)	8 (6%)	0	100	100
12	2Q	139/141 (99%)	125 (90%)	14 (10%)	0	100	100
13	1R	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
13	2R	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
14	1S	108/112 (96%)	106 (98%)	2 (2%)	0	100	100
14	2S	108/112 (96%)	97 (90%)	10 (9%)	1 (1%)	17	25
15	1T	129/146 (88%)	121 (94%)	6 (5%)	2 (2%)	9	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	2T	129/146 (88%)	121 (94%)	8 (6%)	0	100	100
16	1U	114/118 (97%)	114 (100%)	0	0	100	100
16	2U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
17	1V	99/101 (98%)	93 (94%)	4 (4%)	2 (2%)	7	9
17	2V	99/101 (98%)	91 (92%)	7 (7%)	1 (1%)	15	23
18	1W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
18	2W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
19	1X	93/96 (97%)	90 (97%)	2 (2%)	1 (1%)	14	20
19	2X	93/96 (97%)	88 (95%)	4 (4%)	1 (1%)	14	20
20	1Y	105/110 (96%)	97 (92%)	8 (8%)	0	100	100
20	2Y	105/110 (96%)	95 (90%)	10 (10%)	0	100	100
21	1Z	148/206 (72%)	135 (91%)	11 (7%)	2 (1%)	11	15
21	2Z	156/206 (76%)	127 (81%)	29 (19%)	0	100	100
22	10	81/85 (95%)	79 (98%)	2 (2%)	0	100	100
22	20	81/85 (95%)	78 (96%)	3 (4%)	0	100	100
23	11	95/98 (97%)	91 (96%)	3 (3%)	1 (1%)	14	20
23	21	95/98 (97%)	91 (96%)	3 (3%)	1 (1%)	14	20
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	68 (100%)	0	0	100	100
25	13	57/60 (95%)	57 (100%)	0	0	100	100
25	23	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
26	14	67/71 (94%)	54 (81%)	8 (12%)	5 (8%)	1	0
26	24	67/71 (94%)	50 (75%)	14 (21%)	3 (4%)	2	2
27	15	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	25	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
28	16	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
28	26	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
29	17	46/49 (94%)	46 (100%)	0	0	100	100
29	27	46/49 (94%)	46 (100%)	0	0	100	100
30	18	62/65 (95%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	61 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	35 (100%)	0	0	100	100
33	1b	229/256 (90%)	195 (85%)	28 (12%)	6 (3%)	5	5
33	2b	229/256 (90%)	195 (85%)	30 (13%)	4 (2%)	9	11
34	1c	204/239 (85%)	188 (92%)	16 (8%)	0	100	100
34	2c	204/239 (85%)	176 (86%)	27 (13%)	1 (0%)	29	41
35	1d	206/209 (99%)	189 (92%)	16 (8%)	1 (0%)	29	41
35	2d	206/209 (99%)	190 (92%)	16 (8%)	0	100	100
36	1e	146/162 (90%)	132 (90%)	11 (8%)	3 (2%)	7	8
36	2e	146/162 (90%)	132 (90%)	13 (9%)	1 (1%)	22	32
37	1f	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
37	2f	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
38	1g	153/156 (98%)	136 (89%)	15 (10%)	2 (1%)	12	17
38	2g	153/156 (98%)	132 (86%)	16 (10%)	5 (3%)	4	3
39	1h	135/138 (98%)	129 (96%)	6 (4%)	0	100	100
39	2h	135/138 (98%)	128 (95%)	6 (4%)	1 (1%)	22	32
40	1i	125/128 (98%)	110 (88%)	13 (10%)	2 (2%)	9	13
40	2i	125/128 (98%)	106 (85%)	19 (15%)	0	100	100
41	1j	95/105 (90%)	84 (88%)	7 (7%)	4 (4%)	3	2
41	2j	94/105 (90%)	79 (84%)	13 (14%)	2 (2%)	7	8
42	1k	112/129 (87%)	99 (88%)	11 (10%)	2 (2%)	8	10
42	2k	112/129 (87%)	100 (89%)	11 (10%)	1 (1%)	17	25
43	1l	119/132 (90%)	113 (95%)	6 (5%)	0	100	100
43	2l	119/132 (90%)	108 (91%)	9 (8%)	2 (2%)	9	11
44	1m	121/126 (96%)	104 (86%)	15 (12%)	2 (2%)	9	11
44	2m	120/126 (95%)	103 (86%)	15 (12%)	2 (2%)	9	11
45	1n	58/61 (95%)	54 (93%)	4 (7%)	0	100	100
45	2n	58/61 (95%)	54 (93%)	3 (5%)	1 (2%)	9	11
46	1o	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
46	2o	86/89 (97%)	79 (92%)	7 (8%)	0	100	100
47	1p	80/88 (91%)	77 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	2p	80/88 (91%)	71 (89%)	8 (10%)	1 (1%)	12	17
48	1q	97/105 (92%)	90 (93%)	6 (6%)	1 (1%)	15	23
48	2q	97/105 (92%)	87 (90%)	8 (8%)	2 (2%)	7	8
49	1r	66/88 (75%)	61 (92%)	5 (8%)	0	100	100
49	2r	66/88 (75%)	66 (100%)	0	0	100	100
50	1s	81/93 (87%)	68 (84%)	13 (16%)	0	100	100
50	2s	81/93 (87%)	65 (80%)	15 (18%)	1 (1%)	13	19
51	1t	94/106 (89%)	81 (86%)	10 (11%)	3 (3%)	4	3
51	2t	94/106 (89%)	83 (88%)	9 (10%)	2 (2%)	7	8
52	1u	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
52	2u	21/27 (78%)	18 (86%)	3 (14%)	0	100	100
56	1z	2/5 (40%)	1 (50%)	1 (50%)	0	100	100
56	2z	1/5 (20%)	1 (100%)	0	0	100	100
All	All	11371/12138 (94%)	10427 (92%)	842 (7%)	102 (1%)	17	25

All (102) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	1P	29	LYS
21	1Z	53	ILE
23	11	3	LYS
33	1b	17	PHE
40	1i	54	ASP
44	1m	67	GLU
44	1m	107	ALA
11	2P	29	LYS
11	2P	36	LYS
33	2b	17	PHE
33	2b	123	ALA
38	2g	80	VAL
44	2m	67	GLU
48	2q	68	ARG
50	2s	81	ARG
26	14	47	GLN
26	14	49	PHE
26	14	53	GLU
26	14	62	ARG

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Mol	Chain	Res	Type
33	1b	8	LYS
33	1b	126	GLU
38	1g	52	GLU
41	1j	79	ARG
42	1k	49	GLY
5	2F	130	ALA
6	2G	42	GLY
6	2G	43	LEU
6	2G	181	ARG
11	2P	38	GLN
17	2V	79	VAL
26	24	3	GLU
26	24	45	GLY
33	2b	20	GLU
34	2c	54	ARG
38	2g	55	GLY
41	2j	79	ARG
43	2l	91	LYS
44	2m	106	ASN
48	2q	67	LYS
4	1E	28	ALA
4	1E	52	LEU
5	1F	130	ALA
11	1P	38	GLN
15	1T	55	ASN
33	1b	231	GLU
42	1k	74	ALA
48	1q	68	ARG
4	2E	52	LEU
5	2F	21	ALA
5	2F	195	ASP
9	2N	2	LYS
14	2S	84	GLN
19	2X	93	GLU
43	2l	105	TYR
47	2p	52	ASP
51	2t	47	GLY
7	1H	126	PRO
8	1I	10	GLU
9	1N	2	LYS
17	1V	53	GLU
33	1b	124	SER

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Mol	Chain	Res	Type
38	1g	79	ARG
41	1j	78	ASN
51	1t	47	GLY
6	2G	50	ALA
11	2P	45	LEU
26	24	47	GLN
39	2h	133	LEU
41	2j	78	ASN
42	2k	49	GLY
6	1G	43	LEU
11	1P	45	LEU
17	1V	79	VAL
51	1t	96	GLY
7	2H	55	PRO
7	2H	126	PRO
8	2I	40	THR
23	21	3	LYS
38	2g	52	GLU
19	1X	2	LYS
36	1e	86	ALA
40	1i	40	LEU
5	2F	166	ALA
6	2G	24	GLY
36	2e	69	VAL
38	2g	39	ALA
51	2t	102	GLY
15	1T	37	GLY
21	1Z	120	ILE
35	1d	88	VAL
11	2P	44	GLY
41	1j	77	PRO
51	1t	98	PRO
26	14	56	VAL
36	1e	85	GLY
33	2b	125	PRO
38	2g	130	GLY
41	1j	91	PRO
11	2P	122	PRO
36	1e	69	VAL
45	2n	14	PRO
33	1b	125	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	215/218 (99%)	206 (96%)	9 (4%)	30	47
3	2D	215/218 (99%)	203 (94%)	12 (6%)	21	34
4	1E	164/166 (99%)	157 (96%)	7 (4%)	29	46
4	2E	164/166 (99%)	154 (94%)	10 (6%)	18	30
5	1F	160/166 (96%)	145 (91%)	15 (9%)	8	13
5	2F	159/166 (96%)	147 (92%)	12 (8%)	13	21
6	1G	143/156 (92%)	132 (92%)	11 (8%)	13	20
6	2G	143/156 (92%)	127 (89%)	16 (11%)	6	8
7	1H	144/148 (97%)	133 (92%)	11 (8%)	13	20
7	2H	144/148 (97%)	131 (91%)	13 (9%)	9	14
8	1I	113/124 (91%)	94 (83%)	19 (17%)	2	2
8	2I	105/124 (85%)	86 (82%)	19 (18%)	1	2
9	1N	118/119 (99%)	113 (96%)	5 (4%)	30	47
9	2N	118/119 (99%)	114 (97%)	4 (3%)	37	56
10	1O	100/100 (100%)	97 (97%)	3 (3%)	41	61
10	2O	100/100 (100%)	97 (97%)	3 (3%)	41	61
11	1P	115/116 (99%)	105 (91%)	10 (9%)	10	15
11	2P	115/116 (99%)	107 (93%)	8 (7%)	15	24
12	1Q	111/111 (100%)	106 (96%)	5 (4%)	27	44
12	2Q	111/111 (100%)	105 (95%)	6 (5%)	22	36
13	1R	101/101 (100%)	96 (95%)	5 (5%)	24	40
13	2R	101/101 (100%)	97 (96%)	4 (4%)	31	49
14	1S	86/88 (98%)	82 (95%)	4 (5%)	26	42
14	2S	85/88 (97%)	74 (87%)	11 (13%)	4	5
15	1T	115/127 (91%)	111 (96%)	4 (4%)	36	55
15	2T	113/127 (89%)	100 (88%)	13 (12%)	5	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	1U	93/94 (99%)	86 (92%)	7 (8%)	13	21
16	2U	93/94 (99%)	90 (97%)	3 (3%)	39	59
17	1V	80/82 (98%)	75 (94%)	5 (6%)	18	28
17	2V	80/82 (98%)	76 (95%)	4 (5%)	24	40
18	1W	90/92 (98%)	84 (93%)	6 (7%)	16	26
18	2W	90/92 (98%)	86 (96%)	4 (4%)	28	45
19	1X	77/78 (99%)	75 (97%)	2 (3%)	46	66
19	2X	77/78 (99%)	73 (95%)	4 (5%)	23	38
20	1Y	85/91 (93%)	79 (93%)	6 (7%)	14	23
20	2Y	85/91 (93%)	79 (93%)	6 (7%)	14	23
21	1Z	135/179 (75%)	122 (90%)	13 (10%)	8	12
21	2Z	137/179 (76%)	121 (88%)	16 (12%)	5	7
22	10	65/67 (97%)	65 (100%)	0	100	100
22	20	65/67 (97%)	63 (97%)	2 (3%)	40	60
23	11	80/83 (96%)	73 (91%)	7 (9%)	10	15
23	21	80/83 (96%)	74 (92%)	6 (8%)	13	21
24	12	65/67 (97%)	62 (95%)	3 (5%)	27	43
24	22	65/67 (97%)	59 (91%)	6 (9%)	9	13
25	13	51/52 (98%)	46 (90%)	5 (10%)	8	11
25	23	50/52 (96%)	47 (94%)	3 (6%)	19	31
26	14	59/63 (94%)	50 (85%)	9 (15%)	2	3
26	24	53/63 (84%)	39 (74%)	14 (26%)	0	0
27	15	50/52 (96%)	44 (88%)	6 (12%)	5	6
27	25	50/52 (96%)	46 (92%)	4 (8%)	12	18
28	16	51/52 (98%)	45 (88%)	6 (12%)	5	7
28	26	50/52 (96%)	43 (86%)	7 (14%)	3	4
29	17	41/42 (98%)	38 (93%)	3 (7%)	14	22
29	27	41/42 (98%)	37 (90%)	4 (10%)	8	11
30	18	54/55 (98%)	50 (93%)	4 (7%)	13	22
30	28	54/55 (98%)	50 (93%)	4 (7%)	13	22
31	19	34/34 (100%)	32 (94%)	2 (6%)	19	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	29	34/34 (100%)	34 (100%)	0	100	100
33	1b	192/220 (87%)	170 (88%)	22 (12%)	5	7
33	2b	187/220 (85%)	160 (86%)	27 (14%)	3	3
34	1c	142/188 (76%)	130 (92%)	12 (8%)	10	16
34	2c	140/188 (74%)	125 (89%)	15 (11%)	6	9
35	1d	169/181 (93%)	150 (89%)	19 (11%)	6	8
35	2d	173/181 (96%)	159 (92%)	14 (8%)	11	18
36	1e	113/123 (92%)	108 (96%)	5 (4%)	28	45
36	2e	114/123 (93%)	107 (94%)	7 (6%)	18	30
37	1f	84/90 (93%)	78 (93%)	6 (7%)	14	23
37	2f	85/90 (94%)	78 (92%)	7 (8%)	11	17
38	1g	119/127 (94%)	105 (88%)	14 (12%)	5	7
38	2g	120/127 (94%)	109 (91%)	11 (9%)	9	13
39	1h	114/119 (96%)	105 (92%)	9 (8%)	12	19
39	2h	114/119 (96%)	103 (90%)	11 (10%)	8	12
40	1i	90/99 (91%)	80 (89%)	10 (11%)	6	8
40	2i	89/99 (90%)	77 (86%)	12 (14%)	4	4
41	1j	66/92 (72%)	60 (91%)	6 (9%)	9	14
41	2j	69/92 (75%)	60 (87%)	9 (13%)	4	4
42	1k	82/99 (83%)	72 (88%)	10 (12%)	5	6
42	2k	83/99 (84%)	76 (92%)	7 (8%)	11	16
43	1l	96/108 (89%)	91 (95%)	5 (5%)	23	38
43	2l	96/108 (89%)	88 (92%)	8 (8%)	11	17
44	1m	93/101 (92%)	83 (89%)	10 (11%)	6	9
44	2m	92/101 (91%)	78 (85%)	14 (15%)	3	3
45	1n	49/50 (98%)	43 (88%)	6 (12%)	5	6
45	2n	49/50 (98%)	47 (96%)	2 (4%)	30	48
46	1o	78/80 (98%)	71 (91%)	7 (9%)	9	14
46	2o	78/80 (98%)	73 (94%)	5 (6%)	17	28
47	1p	69/74 (93%)	63 (91%)	6 (9%)	10	15
47	2p	68/74 (92%)	65 (96%)	3 (4%)	28	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	1q	94/97 (97%)	89 (95%)	5 (5%)	22	37
48	2q	94/97 (97%)	87 (93%)	7 (7%)	13	22
49	1r	59/77 (77%)	53 (90%)	6 (10%)	7	10
49	2r	59/77 (77%)	51 (86%)	8 (14%)	3	4
50	1s	69/80 (86%)	62 (90%)	7 (10%)	7	11
50	2s	67/80 (84%)	59 (88%)	8 (12%)	5	6
51	1t	70/82 (85%)	65 (93%)	5 (7%)	14	23
51	2t	70/82 (85%)	67 (96%)	3 (4%)	29	46
52	1u	18/22 (82%)	16 (89%)	2 (11%)	6	8
52	2u	18/22 (82%)	18 (100%)	0	100	100
56	1z	3/3 (100%)	3 (100%)	0	100	100
56	2z	2/3 (67%)	2 (100%)	0	100	100
All	All	9308/10070 (92%)	8548 (92%)	760 (8%)	11	17

All (760) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	3	VAL
3	1D	14	ARG
3	1D	22	SER
3	1D	32	SER
3	1D	99	ASP
3	1D	142	VAL
3	1D	154	LYS
3	1D	242	ARG
3	1D	260	ARG
4	1E	12	THR
4	1E	47	VAL
4	1E	61	ARG
4	1E	78	LEU
4	1E	89	ASP
4	1E	116	VAL
4	1E	184	VAL
5	1F	33	LEU
5	1F	57	VAL
5	1F	70	THR
5	1F	72	ARG
5	1F	74	ARG

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Mol	Chain	Res	Type
5	1F	88	VAL
5	1F	106	ARG
5	1F	140	LEU
5	1F	144	LYS
5	1F	158	THR
5	1F	162	LEU
5	1F	168	ARG
5	1F	175	THR
5	1F	192	LEU
5	1F	197	ASP
6	1G	3	LEU
6	1G	7	LEU
6	1G	8	LYS
6	1G	21	ARG
6	1G	31	VAL
6	1G	35	GLU
6	1G	36	LYS
6	1G	43	LEU
6	1G	132	ASN
6	1G	148	MET
6	1G	159	VAL
7	1H	16	SER
7	1H	57	ASP
7	1H	76	VAL
7	1H	84	SER
7	1H	92	ILE
7	1H	103	LEU
7	1H	116	GLU
7	1H	122	THR
7	1H	127	GLU
7	1H	129	THR
7	1H	149	ARG
8	1I	10	GLU
8	1I	20	ASP
8	1I	27	ARG
8	1I	38	LEU
8	1I	45	LYS
8	1I	47	LEU
8	1I	61	ARG
8	1I	68	LEU
8	1I	76	THR
8	1I	77	LEU

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Mol	Chain	Res	Type
8	1I	85	GLU
8	1I	92	VAL
8	1I	101	LEU
8	1I	116	LEU
8	1I	123	LEU
8	1I	127	VAL
8	1I	129	THR
8	1I	140	LEU
8	1I	142	VAL
9	1N	9	VAL
9	1N	28	THR
9	1N	46	VAL
9	1N	48	MET
9	1N	71	ILE
10	1O	28	SER
10	1O	106	LEU
10	1O	112	MET
11	1P	3	LEU
11	1P	7	ARG
11	1P	86	LYS
11	1P	92	GLU
11	1P	96	THR
11	1P	98	GLU
11	1P	101	VAL
11	1P	114	ILE
11	1P	133	SER
11	1P	147	LEU
12	1Q	1	MET
12	1Q	7	MET
12	1Q	75	THR
12	1Q	98	LYS
12	1Q	133	ARG
13	1R	15	SER
13	1R	36	THR
13	1R	44	LEU
13	1R	100	LEU
13	1R	114	VAL
14	1S	14	VAL
14	1S	49	VAL
14	1S	69	VAL
14	1S	73	LEU
15	1T	28	VAL

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Mol	Chain	Res	Type
15	1T	36	GLU
15	1T	125	ARG
15	1T	128	GLU
16	1U	9	VAL
16	1U	17	ILE
16	1U	31	SER
16	1U	55	ARG
16	1U	59	ARG
16	1U	74	LEU
16	1U	95	LEU
17	1V	10	LYS
17	1V	32	THR
17	1V	61	VAL
17	1V	79	VAL
17	1V	85	LYS
18	1W	4	LYS
18	1W	11	ARG
18	1W	15	ARG
18	1W	24	ILE
18	1W	67	ASP
18	1W	96	ILE
19	1X	75	ASP
19	1X	92	LEU
20	1Y	7	VAL
20	1Y	21	LYS
20	1Y	31	LEU
20	1Y	43	ASN
20	1Y	85	VAL
20	1Y	99	CYS
21	1Z	18	LEU
21	1Z	28	MET
21	1Z	53	ILE
21	1Z	61	LEU
21	1Z	91	LEU
21	1Z	124	ILE
21	1Z	129	SER
21	1Z	132	ASN
21	1Z	139	VAL
21	1Z	154	ASP
21	1Z	169	GLU
21	1Z	170	THR
21	1Z	171	ILE

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Mol	Chain	Res	Type
23	11	3	LYS
23	11	11	ARG
23	11	46	LEU
23	11	59	THR
23	11	65	SER
23	11	66	HIS
23	11	78	LYS
24	12	24	LEU
24	12	53	LEU
24	12	55	ARG
25	13	23	LEU
25	13	35	ARG
25	13	37	LEU
25	13	54	VAL
25	13	60	GLU
26	14	14	ILE
26	14	44	THR
26	14	46	GLN
26	14	49	PHE
26	14	52	THR
26	14	53	GLU
26	14	59	PHE
26	14	63	TYR
26	14	69	LYS
27	15	6	VAL
27	15	35	GLU
27	15	40	LYS
27	15	55	ARG
27	15	57	VAL
27	15	59	GLU
28	16	4	GLU
28	16	5	VAL
28	16	6	ARG
28	16	14	THR
28	16	45	LYS
28	16	47	THR
29	17	24	THR
29	17	43	THR
29	17	46	VAL
30	18	14	VAL
30	18	31	HIS
30	18	34	TRP

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Mol	Chain	Res	Type
30	18	50	LEU
31	19	4	ARG
31	19	10	ILE
33	1b	12	GLU
33	1b	21	ARG
33	1b	23	ARG
33	1b	24	TRP
33	1b	35	GLU
33	1b	39	ILE
33	1b	43	ASP
33	1b	44	LEU
33	1b	54	THR
33	1b	64	ARG
33	1b	78	GLN
33	1b	80	ILE
33	1b	101	MET
33	1b	104	ASN
33	1b	127	ILE
33	1b	189	ASP
33	1b	192	SER
33	1b	200	ILE
33	1b	208	ILE
33	1b	212	GLN
33	1b	215	LEU
33	1b	236	TYR
34	1c	3	ASN
34	1c	17	ASP
34	1c	28	GLN
34	1c	36	ASP
34	1c	77	ILE
34	1c	85	ARG
34	1c	89	GLU
34	1c	98	ASN
34	1c	105	GLU
34	1c	178	LEU
34	1c	195	VAL
34	1c	196	LEU
35	1d	3	ARG
35	1d	19	LEU
35	1d	70	ILE
35	1d	76	ARG
35	1d	77	ASN

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Mol	Chain	Res	Type
35	1d	83	SER
35	1d	86	LYS
35	1d	127	THR
35	1d	135	LEU
35	1d	138	TYR
35	1d	140	VAL
35	1d	144	ASP
35	1d	158	ILE
35	1d	170	VAL
35	1d	175	SER
35	1d	177	ASP
35	1d	178	VAL
35	1d	184	LYS
35	1d	194	LEU
36	1e	12	LEU
36	1e	41	VAL
36	1e	45	PHE
36	1e	68	GLU
36	1e	79	GLU
37	1f	36	ARG
37	1f	70	ASP
37	1f	75	LEU
37	1f	78	GLU
37	1f	91	VAL
37	1f	93	SER
38	1g	21	VAL
38	1g	24	THR
38	1g	27	ILE
38	1g	32	ARG
38	1g	41	ARG
38	1g	50	ILE
38	1g	59	LEU
38	1g	61	VAL
38	1g	72	ARG
38	1g	85	TYR
38	1g	94	ARG
38	1g	104	LEU
38	1g	114	ARG
38	1g	115	ARG
39	1h	33	GLU
39	1h	39	LEU
39	1h	51	VAL

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Mol	Chain	Res	Type
39	1h	52	ASP
39	1h	54	ASP
39	1h	77	GLU
39	1h	109	ILE
39	1h	112	LEU
39	1h	133	LEU
40	1i	25	LYS
40	1i	34	ASN
40	1i	50	LEU
40	1i	53	VAL
40	1i	88	TYR
40	1i	89	ASN
40	1i	96	LEU
40	1i	103	THR
40	1i	111	ARG
40	1i	128	ARG
41	1j	17	ASP
41	1j	35	SER
41	1j	81	THR
41	1j	92	THR
41	1j	94	VAL
41	1j	100	THR
42	1k	14	VAL
42	1k	31	THR
42	1k	48	ILE
42	1k	80	VAL
42	1k	87	THR
42	1k	96	ARG
42	1k	104	GLN
42	1k	107	SER
42	1k	109	VAL
42	1k	117	ASN
43	1l	18	VAL
43	1l	33	ARG
43	1l	36	VAL
43	1l	46	LYS
43	1l	112	ASP
44	1m	3	ARG
44	1m	4	ILE
44	1m	17	VAL
44	1m	43	THR
44	1m	57	ARG

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Mol	Chain	Res	Type
44	1m	64	TRP
44	1m	70	LEU
44	1m	106	ASN
44	1m	109	THR
44	1m	121	LYS
45	1n	3	ARG
45	1n	9	LYS
45	1n	13	THR
45	1n	33	VAL
45	1n	56	VAL
45	1n	60	SER
46	1o	24	SER
46	1o	27	VAL
46	1o	39	LEU
46	1o	47	LYS
46	1o	84	LYS
46	1o	87	ILE
46	1o	88	ARG
47	1p	21	VAL
47	1p	27	LYS
47	1p	43	LYS
47	1p	45	THR
47	1p	62	VAL
47	1p	67	THR
48	1q	9	VAL
48	1q	19	VAL
48	1q	26	GLN
48	1q	45	HIS
48	1q	85	VAL
49	1r	29	PHE
49	1r	31	LEU
49	1r	35	ARG
49	1r	36	ASN
49	1r	54	ARG
49	1r	76	LEU
50	1s	6	LYS
50	1s	12	ASP
50	1s	19	VAL
50	1s	28	LYS
50	1s	37	ARG
50	1s	38	SER
50	1s	41	VAL

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Mol	Chain	Res	Type
51	1t	10	LEU
51	1t	24	LEU
51	1t	37	SER
51	1t	84	LEU
51	1t	86	ARG
52	1u	6	ARG
52	1u	15	ARG
3	2D	3	VAL
3	2D	20	ASP
3	2D	22	SER
3	2D	37	LEU
3	2D	54	ARG
3	2D	88	ARG
3	2D	116	GLN
3	2D	141	VAL
3	2D	142	VAL
3	2D	211	ARG
3	2D	242	ARG
3	2D	253	GLN
4	2E	12	THR
4	2E	33	VAL
4	2E	38	THR
4	2E	41	LYS
4	2E	78	LEU
4	2E	90	THR
4	2E	116	VAL
4	2E	119	ARG
4	2E	145	LYS
4	2E	175	VAL
5	2F	20	LEU
5	2F	23	ASP
5	2F	33	LEU
5	2F	50	SER
5	2F	57	VAL
5	2F	74	ARG
5	2F	145	GLU
5	2F	161	GLU
5	2F	162	LEU
5	2F	175	THR
5	2F	183	VAL
5	2F	195	ASP
6	2G	4	ASP

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Mol	Chain	Res	Type
6	2G	19	LEU
6	2G	28	VAL
6	2G	43	LEU
6	2G	45	GLU
6	2G	53	LEU
6	2G	59	GLU
6	2G	60	LEU
6	2G	79	ASN
6	2G	91	ARG
6	2G	109	VAL
6	2G	133	LEU
6	2G	140	ILE
6	2G	148	MET
6	2G	165	THR
6	2G	170	ARG
7	2H	7	LEU
7	2H	15	VAL
7	2H	24	VAL
7	2H	45	VAL
7	2H	57	ASP
7	2H	76	VAL
7	2H	88	LEU
7	2H	122	THR
7	2H	127	GLU
7	2H	129	THR
7	2H	130	ARG
7	2H	134	SER
7	2H	160	LYS
8	2I	2	LYS
8	2I	12	LEU
8	2I	14	ASP
8	2I	38	LEU
8	2I	58	LEU
8	2I	61	ARG
8	2I	69	LYS
8	2I	75	LEU
8	2I	82	ARG
8	2I	85	GLU
8	2I	87	LYS
8	2I	89	TYR
8	2I	96	ASP
8	2I	117	GLU

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Mol	Chain	Res	Type
8	2I	123	LEU
8	2I	129	THR
8	2I	143	SER
8	2I	144	VAL
8	2I	145	VAL
9	2N	28	THR
9	2N	48	MET
9	2N	73	THR
9	2N	83	LYS
10	2O	32	TYR
10	2O	96	THR
10	2O	116	SER
11	2P	3	LEU
11	2P	7	ARG
11	2P	86	LYS
11	2P	95	VAL
11	2P	98	GLU
11	2P	101	VAL
11	2P	133	SER
11	2P	135	LEU
12	2Q	1	MET
12	2Q	10	ARG
12	2Q	21	THR
12	2Q	75	THR
12	2Q	106	VAL
12	2Q	110	THR
13	2R	36	THR
13	2R	44	LEU
13	2R	100	LEU
13	2R	114	VAL
14	2S	12	PHE
14	2S	25	ARG
14	2S	26	LEU
14	2S	27	SER
14	2S	43	GLU
14	2S	58	LEU
14	2S	63	THR
14	2S	76	LYS
14	2S	84	GLN
14	2S	103	GLU
14	2S	110	LEU
15	2T	9	LEU

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Mol	Chain	Res	Type
15	2T	17	THR
15	2T	18	ASP
15	2T	39	ARG
15	2T	57	PHE
15	2T	64	ARG
15	2T	67	SER
15	2T	72	VAL
15	2T	87	ASP
15	2T	89	VAL
15	2T	96	ARG
15	2T	102	ILE
15	2T	113	LYS
16	2U	5	LYS
16	2U	74	LEU
16	2U	95	LEU
17	2V	46	VAL
17	2V	52	VAL
17	2V	79	VAL
17	2V	98	GLU
18	2W	4	LYS
18	2W	11	ARG
18	2W	17	VAL
18	2W	67	ASP
19	2X	35	THR
19	2X	57	LEU
19	2X	81	VAL
19	2X	92	LEU
20	2Y	1	MET
20	2Y	3	VAL
20	2Y	5	MET
20	2Y	30	VAL
20	2Y	97	ARG
20	2Y	99	CYS
21	2Z	27	VAL
21	2Z	42	VAL
21	2Z	67	LEU
21	2Z	70	LEU
21	2Z	71	VAL
21	2Z	81	ARG
21	2Z	91	LEU
21	2Z	100	VAL
21	2Z	121	HIS

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Mol	Chain	Res	Type
21	2Z	128	VAL
21	2Z	136	PHE
21	2Z	144	LEU
21	2Z	154	ASP
21	2Z	170	THR
21	2Z	171	ILE
21	2Z	174	VAL
22	20	14	ARG
22	20	40	GLN
23	21	11	ARG
23	21	40	ARG
23	21	59	THR
23	21	65	SER
23	21	80	LEU
23	21	89	GLU
24	22	4	SER
24	22	19	VAL
24	22	24	LEU
24	22	32	LEU
24	22	53	LEU
24	22	70	GLN
25	23	31	LEU
25	23	35	ARG
25	23	54	VAL
26	24	3	GLU
26	24	22	ILE
26	24	24	THR
26	24	26	SER
26	24	27	THR
26	24	33	VAL
26	24	34	GLU
26	24	37	SER
26	24	48	ARG
26	24	50	VAL
26	24	59	PHE
26	24	63	TYR
26	24	67	TYR
26	24	68	ARG
27	25	6	VAL
27	25	33	CYS
27	25	35	GLU
27	25	55	ARG

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Mol	Chain	Res	Type
28	26	7	ILE
28	26	9	LEU
28	26	14	THR
28	26	19	ARG
28	26	20	ASN
28	26	32	ASN
28	26	48	VAL
29	27	1	MET
29	27	41	ARG
29	27	43	THR
29	27	46	VAL
30	28	23	VAL
30	28	31	HIS
30	28	34	TRP
30	28	50	LEU
33	2b	8	LYS
33	2b	9	GLU
33	2b	16	HIS
33	2b	24	TRP
33	2b	35	GLU
33	2b	48	MET
33	2b	52	GLU
33	2b	68	ILE
33	2b	76	GLN
33	2b	82	ARG
33	2b	83	MET
33	2b	107	THR
33	2b	110	GLN
33	2b	112	VAL
33	2b	115	LEU
33	2b	117	GLU
33	2b	127	ILE
33	2b	142	LEU
33	2b	157	ARG
33	2b	164	VAL
33	2b	168	THR
33	2b	185	ILE
33	2b	187	LEU
33	2b	189	ASP
33	2b	215	LEU
33	2b	224	GLN
33	2b	236	TYR

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Mol	Chain	Res	Type
34	2c	16	ARG
34	2c	26	LYS
34	2c	30	ARG
34	2c	32	LEU
34	2c	69	HIS
34	2c	91	LEU
34	2c	101	LEU
34	2c	115	LEU
34	2c	116	VAL
34	2c	132	ARG
34	2c	161	GLU
34	2c	172	ARG
34	2c	190	ARG
34	2c	192	THR
34	2c	196	LEU
35	2d	5	ILE
35	2d	52	SER
35	2d	58	LEU
35	2d	76	ARG
35	2d	78	LEU
35	2d	86	LYS
35	2d	96	LEU
35	2d	118	ARG
35	2d	127	THR
35	2d	135	LEU
35	2d	150	GLU
35	2d	155	LEU
35	2d	158	ILE
35	2d	193	ASP
36	2e	13	ILE
36	2e	51	VAL
36	2e	83	GLU
36	2e	87	SER
36	2e	118	ILE
36	2e	150	ARG
36	2e	152	ARG
37	2f	30	LEU
37	2f	63	TYR
37	2f	69	GLU
37	2f	81	ILE
37	2f	83	ASP
37	2f	92	LYS

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Mol	Chain	Res	Type
37	2f	95	GLU
38	2g	6	ARG
38	2g	9	VAL
38	2g	21	VAL
38	2g	27	ILE
38	2g	45	ASP
38	2g	53	LYS
38	2g	79	ARG
38	2g	85	TYR
38	2g	98	SER
38	2g	114	ARG
38	2g	139	GLU
39	2h	25	ASP
39	2h	29	SER
39	2h	48	TYR
39	2h	51	VAL
39	2h	52	ASP
39	2h	54	ASP
39	2h	99	GLU
39	2h	109	ILE
39	2h	112	LEU
39	2h	119	LEU
39	2h	133	LEU
40	2i	12	GLU
40	2i	27	THR
40	2i	40	LEU
40	2i	56	LEU
40	2i	64	THR
40	2i	65	VAL
40	2i	66	ARG
40	2i	88	TYR
40	2i	89	ASN
40	2i	102	LEU
40	2i	103	THR
40	2i	113	LYS
41	2j	23	ILE
41	2j	38	ILE
41	2j	55	LYS
41	2j	66	ARG
41	2j	67	THR
41	2j	81	THR
41	2j	97	GLU

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Mol	Chain	Res	Type
41	2j	98	ILE
41	2j	100	THR
42	2k	21	ILE
42	2k	41	THR
42	2k	43	SER
42	2k	81	ASP
42	2k	87	THR
42	2k	105	VAL
42	2k	107	SER
43	2l	33	ARG
43	2l	34	ARG
43	2l	36	VAL
43	2l	39	VAL
43	2l	40	VAL
43	2l	62	SER
43	2l	97	ARG
43	2l	117	ARG
44	2m	32	GLU
44	2m	47	ASP
44	2m	49	THR
44	2m	50	GLU
44	2m	57	ARG
44	2m	70	LEU
44	2m	90	LEU
44	2m	94	ARG
44	2m	102	ARG
44	2m	103	THR
44	2m	106	ASN
44	2m	110	ARG
44	2m	117	VAL
44	2m	121	LYS
45	2n	3	ARG
45	2n	33	VAL
46	2o	3	ILE
46	2o	7	GLU
46	2o	13	GLN
46	2o	27	VAL
46	2o	60	VAL
47	2p	20	VAL
47	2p	42	ARG
47	2p	67	THR
48	2q	5	VAL

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Mol	Chain	Res	Type
48	2q	36	ILE
48	2q	52	LYS
48	2q	60	ILE
48	2q	63	ARG
48	2q	84	LEU
48	2q	96	GLU
49	2r	31	LEU
49	2r	37	VAL
49	2r	47	THR
49	2r	54	ARG
49	2r	56	THR
49	2r	69	THR
49	2r	82	THR
49	2r	87	ARG
50	2s	16	LEU
50	2s	27	GLU
50	2s	37	ARG
50	2s	45	VAL
50	2s	48	THR
50	2s	49	ILE
50	2s	51	VAL
50	2s	57	HIS
51	2t	15	ARG
51	2t	71	THR
51	2t	75	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (116) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	116	GLN
3	1D	126	GLN
3	1D	166	GLN
4	1E	48	GLN
4	1E	121	ASN
5	1F	8	GLN
5	1F	69	HIS
6	1G	26	GLN
6	1G	132	ASN
8	1I	133	HIS
10	1O	3	GLN
12	1Q	12	GLN
13	1R	13	HIS

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Mol	Chain	Res	Type
13	1R	31	HIS
13	1R	71	GLN
15	1T	58	ASN
19	1X	31	HIS
19	1X	82	GLN
20	1Y	6	HIS
21	1Z	32	HIS
21	1Z	73	GLN
21	1Z	151	HIS
22	10	35	ASN
24	12	46	GLN
25	13	32	GLN
33	1b	40	HIS
33	1b	78	GLN
34	1c	6	HIS
34	1c	162	GLN
34	1c	170	GLN
35	1d	116	GLN
35	1d	123	HIS
35	1d	125	HIS
36	1e	20	GLN
36	1e	78	HIS
36	1e	141	GLN
37	1f	13	ASN
37	1f	73	ASN
37	1f	100	ASN
38	1g	13	GLN
38	1g	28	ASN
38	1g	68	ASN
39	1h	15	ASN
40	1i	31	GLN
40	1i	34	ASN
40	1i	58	HIS
40	1i	89	ASN
40	1i	124	GLN
41	1j	56	HIS
43	1l	99	HIS
44	1m	92	HIS
46	1o	9	GLN
46	1o	46	HIS
47	1p	14	ASN
49	1r	63	GLN

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Mol	Chain	Res	Type
50	1s	83	HIS
51	1t	42	GLN
3	2D	87	ASN
3	2D	116	GLN
4	2E	48	GLN
5	2F	69	HIS
8	2I	74	ASN
8	2I	133	HIS
10	2O	5	GLN
10	2O	90	GLN
12	2Q	12	GLN
13	2R	71	GLN
14	2S	38	GLN
15	2T	84	GLN
19	2X	31	HIS
19	2X	82	GLN
21	2Z	32	HIS
21	2Z	50	GLN
21	2Z	55	HIS
21	2Z	73	GLN
21	2Z	151	HIS
25	23	32	GLN
31	29	20	HIS
33	2b	76	GLN
33	2b	94	ASN
33	2b	95	GLN
33	2b	135	GLN
34	2c	98	ASN
34	2c	162	GLN
35	2d	116	GLN
35	2d	119	GLN
35	2d	123	HIS
35	2d	125	HIS
35	2d	161	ASN
37	2f	32	ASN
37	2f	64	GLN
37	2f	73	ASN
37	2f	94	GLN
37	2f	100	ASN
38	2g	11	GLN
38	2g	28	ASN
38	2g	37	ASN

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Mol	Chain	Res	Type
38	2g	86	GLN
39	2h	15	ASN
40	2i	3	GLN
40	2i	31	GLN
40	2i	58	HIS
40	2i	89	ASN
41	2j	21	GLN
41	2j	33	GLN
41	2j	62	HIS
41	2j	68	HIS
42	2k	104	GLN
42	2k	117	ASN
43	2l	99	HIS
44	2m	77	ASN
46	2o	9	GLN
49	2r	63	GLN
50	2s	69	HIS
50	2s	83	HIS
51	2t	75	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2863/2915 (98%)	439 (15%)	27 (0%)
1	2A	2790/2915 (95%)	449 (16%)	25 (0%)
2	1B	119/121 (98%)	13 (10%)	0
2	2B	118/121 (97%)	23 (19%)	0
32	1a	1494/1521 (98%)	237 (15%)	0
32	2a	1498/1521 (98%)	275 (18%)	0
53	1v	12/24 (50%)	0	0
53	2v	12/24 (50%)	0	0
54	1w	70/76 (92%)	21 (30%)	0
54	2w	67/76 (88%)	23 (34%)	0
55	1x	75/77 (97%)	8 (10%)	0
55	2x	75/77 (97%)	10 (13%)	0
57	1y	71/76 (93%)	25 (35%)	0
57	2y	69/76 (90%)	19 (27%)	0
All	All	9333/9620 (97%)	1542 (16%)	52 (0%)

All (1542) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	10	G
1	1A	11	G
1	1A	12	U
1	1A	15	G
1	1A	34	C
1	1A	36	G
1	1A	45	C
1	1A	61	G
1	1A	63	U
1	1A	71	A
1	1A	72	U
1	1A	74	A
1	1A	75	G
1	1A	84	A
1	1A	118	A
1	1A	119	A
1	1A	120	U
1	1A	151	C
1	1A	154	G
1	1A	154(A)	C
1	1A	181	A
1	1A	182	A
1	1A	196	A
1	1A	205	G
1	1A	214	G
1	1A	215	G
1	1A	216	A
1	1A	221	A
1	1A	222	A
1	1A	225	A
1	1A	229	A
1	1A	233	A
1	1A	248	G
1	1A	271(B)	C
1	1A	271(C)	C
1	1A	271(K)	U
1	1A	271(L)	U
1	1A	271(M)	G
1	1A	271(O)	C
1	1A	271(S)	G
1	1A	271(X)	G
1	1A	272(B)	G
1	1A	275	G

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Mol	Chain	Res	Type
1	1A	279	C
1	1A	311	A
1	1A	329	G
1	1A	330	A
1	1A	352	G
1	1A	353	G
1	1A	354	G
1	1A	357	A
1	1A	363	G
1	1A	363(B)	G
1	1A	386	G
1	1A	389	G
1	1A	396	G
1	1A	405	U
1	1A	411	G
1	1A	428	A
1	1A	444	C
1	1A	448	U
1	1A	451	C
1	1A	455	C
1	1A	456	C
1	1A	457	A
1	1A	481	G
1	1A	504	U
1	1A	505	A
1	1A	508	G
1	1A	509	C
1	1A	530	G
1	1A	531	C
1	1A	532	A
1	1A	533	G
1	1A	545	G
1	1A	549	G
1	1A	563	G
1	1A	573	G
1	1A	575	A
1	1A	586	A
1	1A	592	G
1	1A	603	A
1	1A	604	G
1	1A	607	U
1	1A	614(B)	G

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Mol	Chain	Res	Type
1	1A	615	G
1	1A	616	G
1	1A	627	A
1	1A	637	A
1	1A	645	C
1	1A	646	A
1	1A	652(E)	G
1	1A	652(F)	G
1	1A	652(T)	C
1	1A	668	G
1	1A	669	G
1	1A	686	G
1	1A	717	G
1	1A	730	C
1	1A	764	A
1	1A	765	G
1	1A	775	G
1	1A	776	G
1	1A	782	A
1	1A	783	A
1	1A	784	A
1	1A	785	G
1	1A	789	A
1	1A	790	C
1	1A	792	G
1	1A	805	G
1	1A	811	U
1	1A	812	C
1	1A	819	A
1	1A	827	U
1	1A	828	U
1	1A	859	G
1	1A	866	A
1	1A	877	U
1	1A	879	G
1	1A	880	G
1	1A	883	G
1	1A	884	C
1	1A	885	C
1	1A	886	C
1	1A	887	A
1	1A	888	C

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Mol	Chain	Res	Type
1	1A	889	C
1	1A	890	A
1	1A	892	G
1	1A	893	C
1	1A	894	C
1	1A	896	A
1	1A	897	C
1	1A	898	C
1	1A	907	U
1	1A	910	A
1	1A	932	G
1	1A	945	A
1	1A	946	G
1	1A	953	A
1	1A	959	A
1	1A	961	C
1	1A	963	U
1	1A	974	G
1	1A	975	C
1	1A	983	A
1	1A	985	C
1	1A	996	A
1	1A	1012	U
1	1A	1013	C
1	1A	1022	G
1	1A	1026	U
1	1A	1033	U
1	1A	1040	C
1	1A	1044	G
1	1A	1046	A
1	1A	1047	G
1	1A	1054	A
1	1A	1055	G
1	1A	1058	G
1	1A	1059	G
1	1A	1063	G
1	1A	1065	U
1	1A	1068	G
1	1A	1071	G
1	1A	1073	A
1	1A	1074	G
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	1083	U
1	1A	1087	G
1	1A	1088	A
1	1A	1089	G
1	1A	1090	U
1	1A	1093	G
1	1A	1094	U
1	1A	1098	A
1	1A	1099	G
1	1A	1101	U
1	1A	1110	G
1	1A	1111	A
1	1A	1112	G
1	1A	1128	A
1	1A	1135	C
1	1A	1136	G
1	1A	1142	U
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	1205	U
1	1A	1220	A
1	1A	1229	G
1	1A	1248	G
1	1A	1253	A
1	1A	1256	G
1	1A	1271	G
1	1A	1272	A
1	1A	1273	U
1	1A	1281	G
1	1A	1300	U
1	1A	1301	A
1	1A	1303	G
1	1A	1345	C

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Mol	Chain	Res	Type
1	1A	1352	U
1	1A	1359	A
1	1A	1360	A
1	1A	1365	A
1	1A	1380	G
1	1A	1384	A
1	1A	1385	G
1	1A	1395	A
1	1A	1396	U
1	1A	1416	G
1	1A	1417	C
1	1A	1420	U
1	1A	1421	G
1	1A	1428	C
1	1A	1445	A
1	1A	1450	G
1	1A	1455	G
1	1A	1461	G
1	1A	1467	C
1	1A	1482	G
1	1A	1493	C
1	1A	1494	A
1	1A	1497	U
1	1A	1508	A
1	1A	1509	C
1	1A	1509(A)	A
1	1A	1513	C
1	1A	1540	U
1	1A	1554	A
1	1A	1558	A
1	1A	1566	A
1	1A	1569	A
1	1A	1578	U
1	1A	1584	C
1	1A	1586	A
1	1A	1608	A
1	1A	1610	A
1	1A	1616	A
1	1A	1648	C
1	1A	1674	G
1	1A	1700	A
1	1A	1701	A

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Mol	Chain	Res	Type
1	1A	1703	G
1	1A	1722	A
1	1A	1756	G
1	1A	1763	G
1	1A	1764	G
1	1A	1769	G
1	1A	1773	A
1	1A	1780	A
1	1A	1782	C
1	1A	1786	A
1	1A	1791	A
1	1A	1800	C
1	1A	1812	A
1	1A	1816	G
1	1A	1829	A
1	1A	1839	G
1	1A	1847	A
1	1A	1877	A
1	1A	1878	G
1	1A	1889	A
1	1A	1900	A
1	1A	1906	G
1	1A	1927	A
1	1A	1929	G
1	1A	1930	G
1	1A	1937	A
1	1A	1938	A
1	1A	1955	U
1	1A	1960	A
1	1A	1963	U
1	1A	1967	C
1	1A	1970	A
1	1A	1971	A
1	1A	1972	A
1	1A	1992	G
1	1A	1993	U
1	1A	1997	G
1	1A	2020	A
1	1A	2023	G
1	1A	2031	A
1	1A	2032	G
1	1A	2033	A

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Mol	Chain	Res	Type
1	1A	2039	C
1	1A	2043	C
1	1A	2055	C
1	1A	2056	G
1	1A	2060	A
1	1A	2061	G
1	1A	2069	G
1	1A	2108	C
1	1A	2110	G
1	1A	2113	U
1	1A	2116	G
1	1A	2118	U
1	1A	2119	A
1	1A	2120	G
1	1A	2121	G
1	1A	2126	A
1	1A	2127	G
1	1A	2129	C
1	1A	2130	U
1	1A	2131	G
1	1A	2132	U
1	1A	2133	G
1	1A	2134	A
1	1A	2135	A
1	1A	2136	C
1	1A	2137	C
1	1A	2140	C
1	1A	2142	C
1	1A	2143	C
1	1A	2144	U
1	1A	2146	C
1	1A	2150	U
1	1A	2151	G
1	1A	2155	G
1	1A	2156	G
1	1A	2157	G
1	1A	2158	A
1	1A	2159	G
1	1A	2161	C
1	1A	2166	G
1	1A	2171	A
1	1A	2172	U

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Mol	Chain	Res	Type
1	1A	2173	A
1	1A	2174	C
1	1A	2181	G
1	1A	2182	G
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
1	1A	2238	G
1	1A	2239	G
1	1A	2268	A
1	1A	2269	A
1	1A	2283	C
1	1A	2286	A
1	1A	2287	A
1	1A	2289	G
1	1A	2305	A
1	1A	2308	G
1	1A	2309	A
1	1A	2312	U
1	1A	2320	A
1	1A	2325	G
1	1A	2334	G
1	1A	2336	A
1	1A	2347	C
1	1A	2361	A
1	1A	2379	G
1	1A	2383	G
1	1A	2385	C
1	1A	2396	G
1	1A	2400	G
1	1A	2406	U
1	1A	2422	A
1	1A	2423	U
1	1A	2424	C
1	1A	2425	A
1	1A	2428	G

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Mol	Chain	Res	Type
1	1A	2429	G
1	1A	2430	A
1	1A	2431	U
1	1A	2435	A
1	1A	2439	A
1	1A	2441	C
1	1A	2447	G
1	1A	2448	A
1	1A	2468	G
1	1A	2476	A
1	1A	2478	A
1	1A	2491	U
1	1A	2502	G
1	1A	2505	G
1	1A	2518	A
1	1A	2529	G
1	1A	2535	G
1	1A	2554	U
1	1A	2562	U
1	1A	2566	A
1	1A	2567	G
1	1A	2573	C
1	1A	2578	G
1	1A	2602	A
1	1A	2609	U
1	1A	2611	U
1	1A	2612	C
1	1A	2629	A
1	1A	2630	G
1	1A	2654	A
1	1A	2660	A
1	1A	2689	U
1	1A	2690	C
1	1A	2691	C
1	1A	2702	U
1	1A	2703	C
1	1A	2712(A)	A
1	1A	2713	A
1	1A	2714	G
1	1A	2721	A
1	1A	2726	U
1	1A	2733	A

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Mol	Chain	Res	Type
1	1A	2757	A
1	1A	2765	A
1	1A	2778	A
1	1A	2783	G
1	1A	2790	A
1	1A	2791	C
1	1A	2793	G
1	1A	2802	G
1	1A	2803	C
1	1A	2820	A
1	1A	2821	A
1	1A	2835	A
1	1A	2836	U
1	1A	2872	G
1	1A	2876	G
1	1A	2880	C
1	1A	2892	A
1	1A	2894	G
2	1B	2	C
2	1B	13	A
2	1B	25	A
2	1B	35	U
2	1B	45	A
2	1B	50	G
2	1B	56	G
2	1B	57	A
2	1B	67	G
2	1B	73	A
2	1B	85	G
2	1B	92	C
2	1B	110	G
32	1a	7	G
32	1a	9	G
32	1a	31	G
32	1a	32	A
32	1a	39	G
32	1a	47	C
32	1a	48	C
32	1a	51	A
32	1a	52	G
32	1a	61	G
32	1a	73	G

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Mol	Chain	Res	Type
32	1a	77	G
32	1a	79	G
32	1a	91	C
32	1a	98	G
32	1a	101	A
32	1a	116	A
32	1a	121	C
32	1a	131	C
32	1a	142	G
32	1a	144	G
32	1a	145	G
32	1a	147	G
32	1a	163	C
32	1a	164	U
32	1a	174	C
32	1a	180	U
32	1a	182	U
32	1a	189(C)	C
32	1a	189(F)	U
32	1a	189(J)	G
32	1a	195	A
32	1a	197	A
32	1a	202	U
32	1a	203	U
32	1a	204	U
32	1a	247	G
32	1a	251	G
32	1a	266	G
32	1a	267	C
32	1a	289	G
32	1a	321	A
32	1a	328	C
32	1a	332	G
32	1a	347	G
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	384	G
32	1a	397	A

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Mol	Chain	Res	Type
32	1a	398	C
32	1a	406	G
32	1a	412	A
32	1a	413	G
32	1a	422	C
32	1a	423	G
32	1a	424	G
32	1a	429	U
32	1a	439	A
32	1a	441	A
32	1a	442	C
32	1a	451	A
32	1a	452	A
32	1a	461	A
32	1a	470	C
32	1a	483	C
32	1a	485	G
32	1a	496	A
32	1a	498	U
32	1a	509	A
32	1a	510	A
32	1a	511	C
32	1a	518	C
32	1a	531	U
32	1a	532	A
32	1a	533	A
32	1a	547	A
32	1a	559	A
32	1a	560	U
32	1a	561	U
32	1a	568	G
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	577	G
32	1a	592	G
32	1a	596	C
32	1a	607	A
32	1a	630	G
32	1a	653	A
32	1a	665	A
32	1a	666	G

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Mol	Chain	Res	Type
32	1a	671	G
32	1a	672	U
32	1a	673	G
32	1a	687	A
32	1a	688	G
32	1a	723	U
32	1a	731	G
32	1a	734	G
32	1a	738	C
32	1a	749	C
32	1a	755	G
32	1a	777	A
32	1a	792	A
32	1a	793	U
32	1a	794	A
32	1a	806	C
32	1a	815	A
32	1a	816	A
32	1a	817	C
32	1a	821	G
32	1a	828	A
32	1a	840	C
32	1a	841	U
32	1a	851	G
32	1a	860	A
32	1a	870	U
32	1a	874	G
32	1a	902	G
32	1a	914	A
32	1a	916	G
32	1a	926	G
32	1a	927	G
32	1a	932	C
32	1a	934	C
32	1a	936	C
32	1a	942	G
32	1a	950	U
32	1a	960	U
32	1a	961	U
32	1a	968	A
32	1a	969	A
32	1a	971	G

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Mol	Chain	Res	Type
32	1a	972	C
32	1a	974	A
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	992	U
32	1a	993	G
32	1a	997	U
32	1a	1000	U
32	1a	1003	G
32	1a	1005	A
32	1a	1006	C
32	1a	1011	G
32	1a	1020	U
32	1a	1022	G
32	1a	1023	G
32	1a	1025	U
32	1a	1026	G
32	1a	1027	C
32	1a	1028	C
32	1a	1029	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	1035	A
32	1a	1037	C
32	1a	1039	C
32	1a	1044	A
32	1a	1045	C
32	1a	1068	G
32	1a	1081	G
32	1a	1086	U
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1108	G
32	1a	1123	A
32	1a	1124	G
32	1a	1125	U
32	1a	1127	G

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Mol	Chain	Res	Type
32	1a	1132	C
32	1a	1134	G
32	1a	1137	C
32	1a	1138	G
32	1a	1139	G
32	1a	1146	A
32	1a	1152	A
32	1a	1154	G
32	1a	1157	A
32	1a	1159	U
32	1a	1183	A
32	1a	1184	G
32	1a	1196	U
32	1a	1197	G
32	1a	1202	G
32	1a	1213	A
32	1a	1219	U
32	1a	1227	A
32	1a	1236	A
32	1a	1238	A
32	1a	1253	G
32	1a	1256	A
32	1a	1257	U
32	1a	1270	C
32	1a	1275	A
32	1a	1278	U
32	1a	1279	A
32	1a	1280	A
32	1a	1286	A
32	1a	1287	A
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1312	G
32	1a	1320	C
32	1a	1322	C
32	1a	1338	G
32	1a	1346	A
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1363(A)	A

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Mol	Chain	Res	Type
32	1a	1370	G
32	1a	1397	C
32	1a	1419	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1446	U
32	1a	1447	A
32	1a	1456	G
32	1a	1492	A
32	1a	1494	G
32	1a	1503	A
32	1a	1504	G
32	1a	1506	U
32	1a	1517	G
32	1a	1529	G
32	1a	1530	G
54	1w	2	C
54	1w	6	G
54	1w	7	A
54	1w	8	4SU
54	1w	9	A
54	1w	14	A
54	1w	19	G
54	1w	20	U
54	1w	21	A
54	1w	23	A
54	1w	24	G
54	1w	36	A
54	1w	45	U
54	1w	46	G7M
54	1w	47	U
54	1w	48	C
54	1w	62	C
54	1w	67	C
54	1w	68	C
54	1w	73	A
54	1w	74	C
55	1x	5	G
55	1x	7	G
55	1x	9	G
55	1x	21	A
55	1x	47	U

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Mol	Chain	Res	Type
55	1x	61	C
55	1x	63	G
55	1x	64	G
57	1y	5	G
57	1y	6	G
57	1y	9	A
57	1y	13	C
57	1y	14	A
57	1y	19	G
57	1y	20	U
57	1y	21	A
57	1y	29	G
57	1y	35	A
57	1y	39	PSU
57	1y	44	G
57	1y	45	U
57	1y	46	G7M
57	1y	47	U
57	1y	48	C
57	1y	52	G
57	1y	56	C
57	1y	57	G
57	1y	58	A
57	1y	59	U
57	1y	61	C
57	1y	66	U
57	1y	70	G
57	1y	72	C
1	2A	8	A
1	2A	12	U
1	2A	15	G
1	2A	34	C
1	2A	35	G
1	2A	36	G
1	2A	45	C
1	2A	61	G
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	84	A
1	2A	90	U
1	2A	94	C

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Mol	Chain	Res	Type
1	2A	100	G
1	2A	102	G
1	2A	118	A
1	2A	119	A
1	2A	120	U
1	2A	154	G
1	2A	154(A)	C
1	2A	157	U
1	2A	181	A
1	2A	196	A
1	2A	199	A
1	2A	205	G
1	2A	214	G
1	2A	215	G
1	2A	216	A
1	2A	222	A
1	2A	225	A
1	2A	228	A
1	2A	229	A
1	2A	230	U
1	2A	233	A
1	2A	248	G
1	2A	271(J)	C
1	2A	271(K)	U
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	271(O)	C
1	2A	272(B)	G
1	2A	277	C
1	2A	278	A
1	2A	311	A
1	2A	327	G
1	2A	329	G
1	2A	330	A
1	2A	346	A
1	2A	352	G
1	2A	354	G
1	2A	363	G
1	2A	363(B)	G
1	2A	370	G
1	2A	386	G

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Mol	Chain	Res	Type
1	2A	389	G
1	2A	399	G
1	2A	403	U
1	2A	411	G
1	2A	412	A
1	2A	421	U
1	2A	435	C
1	2A	442	G
1	2A	443	A
1	2A	444	C
1	2A	454	A
1	2A	455	C
1	2A	457	A
1	2A	479	A
1	2A	481	G
1	2A	505	A
1	2A	508	G
1	2A	509	C
1	2A	529	A
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	533	G
1	2A	545	G
1	2A	551	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	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	627	A
1	2A	634	C
1	2A	637	A
1	2A	645	C

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Mol	Chain	Res	Type
1	2A	652(B)	A
1	2A	652(C)	G
1	2A	656	G
1	2A	669	G
1	2A	686	G
1	2A	701	G
1	2A	730	C
1	2A	740	U
1	2A	752	A
1	2A	753	C
1	2A	774	A
1	2A	775	G
1	2A	776	G
1	2A	782	A
1	2A	784	A
1	2A	785	G
1	2A	792	G
1	2A	793	A
1	2A	805	G
1	2A	812	C
1	2A	819	A
1	2A	827	U
1	2A	828	U
1	2A	857	C
1	2A	859	G
1	2A	869	G
1	2A	874	G
1	2A	875	G
1	2A	878	A
1	2A	879	G
1	2A	880	G
1	2A	884	C
1	2A	886	C
1	2A	887	A
1	2A	888	C
1	2A	889	C
1	2A	893	C
1	2A	894	C
1	2A	895	U
1	2A	896	A
1	2A	900	A
1	2A	901	A

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Mol	Chain	Res	Type
1	2A	904	C
1	2A	910	A
1	2A	917	A
1	2A	932	G
1	2A	933	A
1	2A	938	G
1	2A	941	A
1	2A	945	A
1	2A	946	G
1	2A	950	G
1	2A	953	A
1	2A	959	A
1	2A	961	C
1	2A	974	G
1	2A	975	C
1	2A	983	A
1	2A	990	A
1	2A	996	A
1	2A	999	U
1	2A	1005	C
1	2A	1012	U
1	2A	1013	C
1	2A	1017	G
1	2A	1021	A
1	2A	1022	G
1	2A	1025	G
1	2A	1026	U
1	2A	1033	U
1	2A	1038	C
1	2A	1039	G
1	2A	1041	C
1	2A	1114	G
1	2A	1116	C
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1139	G
1	2A	1143	A
1	2A	1167	U
1	2A	1171	G
1	2A	1206	G
1	2A	1210	A

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Mol	Chain	Res	Type
1	2A	1211	U
1	2A	1220	A
1	2A	1241	A
1	2A	1248	G
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A
1	2A	1273	U
1	2A	1300	U
1	2A	1301	A
1	2A	1303	G
1	2A	1314	C
1	2A	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	1379	A
1	2A	1384	A
1	2A	1385	G
1	2A	1386	C
1	2A	1416	G
1	2A	1417	C
1	2A	1420	U
1	2A	1421	G
1	2A	1427	A
1	2A	1428	C
1	2A	1437	C
1	2A	1445	A
1	2A	1449	A
1	2A	1450	G
1	2A	1455	G
1	2A	1459	G
1	2A	1460	A
1	2A	1461	G
1	2A	1463	C
1	2A	1467	C
1	2A	1471	A
1	2A	1482	G

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Mol	Chain	Res	Type
1	2A	1486	A
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	1531	C
1	2A	1547	C
1	2A	1558	A
1	2A	1559	G
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1580	A
1	2A	1584	C
1	2A	1608	A
1	2A	1609	A
1	2A	1610	A
1	2A	1616	A
1	2A	1648	C
1	2A	1654	A
1	2A	1667	G
1	2A	1674	G
1	2A	1696	G
1	2A	1700	A
1	2A	1721	G
1	2A	1722	A
1	2A	1740	G
1	2A	1756	G
1	2A	1762	A
1	2A	1763	G
1	2A	1764	G
1	2A	1773	A
1	2A	1780	A
1	2A	1782	C
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1816	G

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Mol	Chain	Res	Type
1	2A	1828	G
1	2A	1829	A
1	2A	1835	G
1	2A	1847	A
1	2A	1848	A
1	2A	1861	G
1	2A	1866	C
1	2A	1877	A
1	2A	1878	G
1	2A	1900	A
1	2A	1906	G
1	2A	1914	C
1	2A	1929	G
1	2A	1930	G
1	2A	1931	U
1	2A	1936	A
1	2A	1938	A
1	2A	1955	U
1	2A	1963	U
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1984	G
1	2A	1992	G
1	2A	1993	U
1	2A	1997	G
1	2A	2020	A
1	2A	2023	G
1	2A	2031	A
1	2A	2033	A
1	2A	2043	C
1	2A	2055	C
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G
1	2A	2069	G
1	2A	2093	G
1	2A	2099	U
1	2A	2110	G
1	2A	2111	C
1	2A	2112	G

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Mol	Chain	Res	Type
1	2A	2116	G
1	2A	2117	A
1	2A	2120	G
1	2A	2122	U
1	2A	2125	G
1	2A	2126	A
1	2A	2127	G
1	2A	2128	C
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	2139	C
1	2A	2140	C
1	2A	2142	C
1	2A	2145	C
1	2A	2149	G
1	2A	2150	U
1	2A	2151	G
1	2A	2155	G
1	2A	2156	G
1	2A	2157	G
1	2A	2158	A
1	2A	2161	C
1	2A	2165	G
1	2A	2166	G
1	2A	2167	U
1	2A	2168	G
1	2A	2172	U
1	2A	2176	A
1	2A	2178	C
1	2A	2183	C
1	2A	2185	C
1	2A	2189	U
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A

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Mol	Chain	Res	Type
1	2A	2225	A
1	2A	2238	G
1	2A	2239	G
1	2A	2275	C
1	2A	2278	A
1	2A	2280	G
1	2A	2283	C
1	2A	2287	A
1	2A	2297	C
1	2A	2298	A
1	2A	2305	A
1	2A	2308	G
1	2A	2319	G
1	2A	2320	A
1	2A	2325	G
1	2A	2327	A
1	2A	2334	G
1	2A	2336	A
1	2A	2347	C
1	2A	2350	C
1	2A	2354	G
1	2A	2366	A
1	2A	2376	A
1	2A	2383	G
1	2A	2385	C
1	2A	2391	G
1	2A	2403	C
1	2A	2406	U
1	2A	2410	G
1	2A	2425	A
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	2459	A
1	2A	2469	A
1	2A	2474	C
1	2A	2476	A
1	2A	2478	A
1	2A	2491	U

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Mol	Chain	Res	Type
1	2A	2494	G
1	2A	2497	A
1	2A	2502	G
1	2A	2505	G
1	2A	2506	U
1	2A	2518	A
1	2A	2520	C
1	2A	2529	G
1	2A	2549	G
1	2A	2554	U
1	2A	2555	U
1	2A	2562	U
1	2A	2566	A
1	2A	2567	G
1	2A	2573	C
1	2A	2574	G
1	2A	2578	G
1	2A	2582	G
1	2A	2585	U
1	2A	2602	A
1	2A	2611	U
1	2A	2612	C
1	2A	2630	G
1	2A	2634	G
1	2A	2645	G
1	2A	2654	A
1	2A	2660	A
1	2A	2689	U
1	2A	2690	C
1	2A	2702	U
1	2A	2703	C
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G
1	2A	2726	U
1	2A	2733	A
1	2A	2748	A
1	2A	2751	G
1	2A	2757	A
1	2A	2758	A
1	2A	2765	A
1	2A	2778	A

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Mol	Chain	Res	Type
1	2A	2789	C
1	2A	2793	G
1	2A	2802	G
1	2A	2803	C
1	2A	2807	G
1	2A	2820	A
1	2A	2821	A
1	2A	2833	G
1	2A	2835	A
1	2A	2836	U
1	2A	2872	G
1	2A	2873	A
1	2A	2892	A
1	2A	2894	G
1	2A	2897	U
2	2B	2	C
2	2B	3	C
2	2B	8	U
2	2B	12	C
2	2B	13	A
2	2B	17	C
2	2B	19	G
2	2B	20	C
2	2B	33	G
2	2B	41	U
2	2B	45	A
2	2B	53	A
2	2B	54	G
2	2B	67	G
2	2B	73	A
2	2B	74	U
2	2B	75	G
2	2B	89	G
2	2B	106	G
2	2B	109	C
2	2B	110	G
2	2B	116	G
2	2B	120	A
32	2a	9	G
32	2a	22	G
32	2a	31	G
32	2a	32	A

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Mol	Chain	Res	Type
32	2a	39	G
32	2a	47	C
32	2a	48	C
32	2a	50	A
32	2a	51	A
32	2a	66	G
32	2a	70	G
32	2a	73	G
32	2a	79	G
32	2a	80	G
32	2a	88	A
32	2a	89	C
32	2a	93	G
32	2a	98	G
32	2a	101	A
32	2a	116	A
32	2a	121	C
32	2a	131	C
32	2a	133	U
32	2a	144	G
32	2a	162	A
32	2a	163	C
32	2a	175	C
32	2a	182	U
32	2a	189(F)	U
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	231	G
32	2a	244	U
32	2a	247	G
32	2a	249	U
32	2a	250	A
32	2a	251	G
32	2a	258	G
32	2a	262	A
32	2a	266	G
32	2a	267	C
32	2a	289	G

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Mol	Chain	Res	Type
32	2a	301	G
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	345	C
32	2a	350	G
32	2a	352	C
32	2a	353	A
32	2a	354	G
32	2a	355	C
32	2a	367	U
32	2a	372	C
32	2a	373	A
32	2a	381	C
32	2a	384	G
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	412	A
32	2a	413	G
32	2a	421	U
32	2a	423	G
32	2a	424	G
32	2a	429	U
32	2a	442	C
32	2a	452	A
32	2a	458	C
32	2a	470	C
32	2a	485	G
32	2a	492	G
32	2a	496	A
32	2a	498	U
32	2a	505	G
32	2a	509	A
32	2a	510	A
32	2a	511	C
32	2a	518	C
32	2a	527	G7M
32	2a	531	U
32	2a	532	A
32	2a	533	A
32	2a	547	A

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Mol	Chain	Res	Type
32	2a	559	A
32	2a	564	C
32	2a	568	G
32	2a	572	A
32	2a	573	A
32	2a	574	A
32	2a	576	G
32	2a	577	G
32	2a	596	C
32	2a	630	G
32	2a	639	G
32	2a	641	U
32	2a	653	A
32	2a	665	A
32	2a	666	G
32	2a	671	G
32	2a	687	A
32	2a	688	G
32	2a	695	A
32	2a	723	U
32	2a	724	G
32	2a	731	G
32	2a	749	C
32	2a	755	G
32	2a	774	G
32	2a	777	A
32	2a	787	A
32	2a	792	A
32	2a	793	U
32	2a	794	A
32	2a	817	C
32	2a	821	G
32	2a	827	U
32	2a	828	A
32	2a	840	C
32	2a	841	U
32	2a	851	G
32	2a	853	G
32	2a	855	G
32	2a	859	A
32	2a	874	G
32	2a	902	G

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Mol	Chain	Res	Type
32	2a	914	A
32	2a	924	C
32	2a	926	G
32	2a	927	G
32	2a	934	C
32	2a	935	A
32	2a	938	A
32	2a	942	G
32	2a	960	U
32	2a	961	U
32	2a	968	A
32	2a	969	A
32	2a	971	G
32	2a	972	C
32	2a	974	A
32	2a	975	A
32	2a	976	G
32	2a	977	A
32	2a	982	U
32	2a	992	U
32	2a	993	G
32	2a	997	U
32	2a	999	C
32	2a	1002	G
32	2a	1003	G
32	2a	1005	A
32	2a	1006	C
32	2a	1009	G
32	2a	1011	G
32	2a	1016	A
32	2a	1020	U
32	2a	1021	G
32	2a	1022	G
32	2a	1023	G
32	2a	1025	U
32	2a	1026	G
32	2a	1027	C
32	2a	1028	C
32	2a	1029	C
32	2a	1030	C
32	2a	1030(A)	G
32	2a	1032	G

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Mol	Chain	Res	Type
32	2a	1033	G
32	2a	1035	A
32	2a	1036	G
32	2a	1037	C
32	2a	1039	C
32	2a	1040	U
32	2a	1043	C
32	2a	1045	C
32	2a	1051	C
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1077	G
32	2a	1079	G
32	2a	1081	G
32	2a	1085	U
32	2a	1086	U
32	2a	1092	A
32	2a	1093	A
32	2a	1094	G
32	2a	1095	U
32	2a	1101	A
32	2a	1105	A
32	2a	1125	U
32	2a	1127	G
32	2a	1129	C
32	2a	1130	A
32	2a	1133	G
32	2a	1136	U
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G
32	2a	1140	C
32	2a	1143	G
32	2a	1144	G
32	2a	1146	A
32	2a	1152	A
32	2a	1157	A
32	2a	1158	C
32	2a	1159	U
32	2a	1160	G
32	2a	1182	G

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Mol	Chain	Res	Type
32	2a	1184	G
32	2a	1186	G
32	2a	1191	A
32	2a	1192	C
32	2a	1193	G
32	2a	1196	U
32	2a	1197	G
32	2a	1201	A
32	2a	1202	G
32	2a	1211	U
32	2a	1212	U
32	2a	1213	A
32	2a	1215	G
32	2a	1227	A
32	2a	1236	A
32	2a	1238	A
32	2a	1240	U
32	2a	1241	G
32	2a	1255	G
32	2a	1256	A
32	2a	1257	U
32	2a	1260	C
32	2a	1264	C
32	2a	1270	C
32	2a	1272	G
32	2a	1273	G
32	2a	1278	U
32	2a	1279	A
32	2a	1280	A
32	2a	1281	U
32	2a	1287	A
32	2a	1302	U
32	2a	1303	C
32	2a	1305	G
32	2a	1316	G
32	2a	1338	G
32	2a	1346	A
32	2a	1347	G
32	2a	1352	C
32	2a	1359	C
32	2a	1363	C
32	2a	1368	G

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Mol	Chain	Res	Type
32	2a	1370	G
32	2a	1380	U
32	2a	1397	C
32	2a	1404	5MC
32	2a	1405	G
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1447	A
32	2a	1452	C
32	2a	1487	G
32	2a	1492	A
32	2a	1504	G
32	2a	1506	U
32	2a	1517	G
32	2a	1529	G
32	2a	1530	G
32	2a	1531	A
32	2a	1532	U
54	2w	4	C
54	2w	6	G
54	2w	8	4SU
54	2w	9	A
54	2w	12	U
54	2w	13	C
54	2w	14	A
54	2w	19	G
54	2w	22	G
54	2w	46	G7M
54	2w	47	U
54	2w	48	C
54	2w	50	U
54	2w	51	U
54	2w	58	A
54	2w	62	C
54	2w	64	A
54	2w	65	G
54	2w	66	U
54	2w	68	C
54	2w	69	G
54	2w	70	G
54	2w	74	C

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Mol	Chain	Res	Type
55	2x	9	G
55	2x	13	C
55	2x	18	G
55	2x	19	G
55	2x	20	U
55	2x	21	A
55	2x	47	U
55	2x	56	C
55	2x	61	C
55	2x	69	C
57	2y	15	G
57	2y	19	G
57	2y	23	A
57	2y	27	G
57	2y	38	A
57	2y	40	C
57	2y	48	C
57	2y	49	C
57	2y	52	G
57	2y	53	G
57	2y	54	5MU
57	2y	56	C
57	2y	58	A
57	2y	59	U
57	2y	65	G
57	2y	68	C
57	2y	69	G
57	2y	70	G
57	2y	73	A

All (52) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	196	A
1	1A	266	G
1	1A	271(J)	C
1	1A	271(K)	U
1	1A	278	A
1	1A	548	A
1	1A	685	A
1	1A	746	A
1	1A	764	A

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Mol	Chain	Res	Type
1	1A	974	G
1	1A	1067	A
1	1A	1174	A
1	1A	1176	G
1	1A	1379	A
1	1A	1442	G
1	1A	1508	A
1	1A	1608	A
1	1A	1992	G
1	1A	2134	A
1	1A	2181	G
1	1A	2183	C
1	1A	2406	U
1	1A	2430	A
1	1A	2439	A
1	1A	2629	A
1	1A	2689	U
1	1A	2756	U
1	2A	196	A
1	2A	228	A
1	2A	266	G
1	2A	271(M)	G
1	2A	277	C
1	2A	528	A
1	2A	752	A
1	2A	827	U
1	2A	856	C
1	2A	900	A
1	2A	1210	A
1	2A	1240	U
1	2A	1420	U
1	2A	1442	G
1	2A	1460	A
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	2335	A
1	2A	2439	A
1	2A	2689	U

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Mol	Chain	Res	Type
1	2A	2756	U

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

88 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	$\#\|Z\| > 2$
55	PSU	2x	55	55	18,21,22	1.33	2 (11%)	22,30,33	1.87	3 (13%)
1	OMU	1A	2552	58,1	19,22,23	1.21	2 (10%)	26,31,34	1.66	4 (15%)
54	5MU	1w	54	54	19,22,23	1.31	3 (15%)	28,32,35	2.13	6 (21%)
57	5MU	1y	54	57	19,22,23	1.43	4 (21%)	28,32,35	1.88	6 (21%)
54	5MU	2w	54	54	19,22,23	1.38	4 (21%)	28,32,35	1.78	5 (17%)
1	5MC	2A	1962	58,1	18,22,23	1.01	2 (11%)	26,32,35	1.15	2 (7%)
57	PSU	1y	39	57	18,21,22	1.33	2 (11%)	22,30,33	1.84	4 (18%)
1	PSU	1A	1911	1	18,21,22	1.33	2 (11%)	22,30,33	1.96	4 (18%)
32	5MC	2a	1407	32	18,22,23	0.91	2 (11%)	26,32,35	1.18	3 (11%)
54	F3N	1w	76	54,1	30,36,37	1.40	5 (16%)	29,51,54	1.20	1 (3%)
57	G7M	1y	46	57	20,26,27	1.35	2 (10%)	17,39,42	0.59	0
32	UR3	2a	1498	32	19,22,23	1.02	0	26,32,35	1.45	1 (3%)
54	PSU	2w	32	54	18,21,22	1.38	2 (11%)	22,30,33	1.74	4 (18%)
54	MIA	2w	37	54	20,27,32	1.87	2 (10%)	22,39,47	1.93	6 (27%)
57	PSU	1y	32	57	18,21,22	1.35	2 (11%)	22,30,33	1.79	4 (18%)
32	MA6	1a	1518	32	19,26,27	0.83	0	18,38,41	1.49	2 (11%)
32	M2G	1a	966	32	20,27,28	1.46	3 (15%)	22,40,43	1.07	2 (9%)
57	PSU	1y	55	57	18,21,22	1.36	2 (11%)	22,30,33	1.88	4 (18%)
1	5MC	1A	1962	1	18,22,23	0.95	2 (11%)	26,32,35	1.14	2 (7%)
55	5MU	1x	54	55	19,22,23	1.41	5 (26%)	28,32,35	1.92	6 (21%)
32	4OC	2a	1402	32	20,23,24	0.75	0	26,32,35	1.22	3 (11%)
32	2MG	1a	1207	32	18,26,27	0.97	1 (5%)	16,38,41	1.07	2 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	5MU	1A	1939	58,1	19,22,23	1.51	6 (31%)	28,32,35	2.19	6 (21%)
1	PSU	1A	2605	1	18,21,22	1.40	3 (16%)	22,30,33	1.98	5 (22%)
1	5MC	2A	1942	1	18,22,23	0.96	1 (5%)	26,32,35	1.14	2 (7%)
32	5MC	2a	1400	32	18,22,23	1.01	2 (11%)	26,32,35	1.19	2 (7%)
1	5MU	2A	1915	1	19,22,23	1.48	5 (26%)	28,32,35	2.06	7 (25%)
55	5MU	2x	54	55	19,22,23	1.40	5 (26%)	28,32,35	2.31	6 (21%)
54	G7M	1w	46	54	20,26,27	1.17	2 (10%)	17,39,42	0.86	0
32	G7M	2a	527	58,32	20,26,27	1.19	2 (10%)	17,39,42	0.51	0
1	OMG	2A	2251	58,55,1	18,26,27	0.94	1 (5%)	19,38,41	1.22	4 (21%)
55	4SU	1x	8	55	18,21,22	2.08	5 (27%)	26,30,33	1.82	6 (23%)
54	F3N	2w	76	54,1	30,36,37	1.46	5 (16%)	29,51,54	1.16	1 (3%)
55	PSU	1x	55	55	18,21,22	1.40	2 (11%)	22,30,33	1.76	3 (13%)
57	PSU	2y	32	57	18,21,22	1.34	2 (11%)	22,30,33	1.85	4 (18%)
32	4OC	1a	1402	32	20,23,24	0.77	0	26,32,35	0.91	1 (3%)
32	MA6	2a	1518	32	19,26,27	0.82	0	18,38,41	1.50	2 (11%)
1	OMG	1A	2251	58,55,1	18,26,27	0.94	1 (5%)	19,38,41	1.19	3 (15%)
32	5MC	1a	1400	32	18,22,23	1.00	2 (11%)	26,32,35	1.18	3 (11%)
55	8AN	2x	76	59,58,56,55	19,24,25	1.23	3 (15%)	13,35,38	1.94	3 (23%)
55	5MC	2x	32	55	18,22,23	0.94	2 (11%)	26,32,35	1.35	5 (19%)
1	5MU	1A	1915	1	19,22,23	1.31	5 (26%)	28,32,35	2.12	7 (25%)
54	G7M	2w	46	54	20,26,27	1.19	1 (5%)	17,39,42	0.89	0
32	MA6	1a	1519	32	19,26,27	0.81	0	18,38,41	1.59	2 (11%)
1	PSU	2A	2605	1	18,21,22	1.31	3 (16%)	22,30,33	2.04	3 (13%)
55	5MC	1x	32	55	18,22,23	0.97	2 (11%)	26,32,35	1.24	2 (7%)
57	MIA	1y	37	57	18,24,32	1.12	2 (11%)	18,35,47	1.20	2 (11%)
32	2MG	2a	1207	32	18,26,27	0.97	1 (5%)	16,38,41	1.10	2 (12%)
57	5MU	2y	54	57	19,22,23	1.52	5 (26%)	28,32,35	1.65	8 (28%)
54	PSU	2w	39	54	18,21,22	1.37	2 (11%)	22,30,33	1.72	4 (18%)
57	PSU	2y	39	42,57	18,21,22	1.35	2 (11%)	22,30,33	1.73	4 (18%)
32	5MC	1a	1407	32	18,22,23	0.91	1 (5%)	26,32,35	1.14	3 (11%)
54	4SU	2w	8	54	18,21,22	1.68	3 (16%)	26,30,33	2.43	5 (19%)
1	5MC	1A	1942	1	18,22,23	0.92	2 (11%)	26,32,35	1.24	2 (7%)
1	2MA	1A	2503	58,1	17,25,26	1.11	2 (11%)	17,37,40	0.90	1 (5%)
54	4SU	1w	8	54	18,21,22	1.88	5 (27%)	26,30,33	1.63	5 (19%)
57	4SU	2y	8	57	18,21,22	1.69	4 (22%)	26,30,33	2.03	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
57	4SU	1y	8	57	18,21,22	1.67	4 (22%)	26,30,33	2.07	5 (19%)
32	PSU	2a	516	32	18,21,22	1.31	2 (11%)	22,30,33	1.85	4 (18%)
1	5MU	2A	1939	1	19,22,23	1.41	6 (31%)	28,32,35	2.10	6 (21%)
1	OMC	2A	1920	1	19,22,23	0.82	0	26,31,34	0.94	0
32	PSU	1a	516	58,32	18,21,22	1.38	2 (11%)	22,30,33	1.78	4 (18%)
54	PSU	2w	55	54	18,21,22	1.35	2 (11%)	22,30,33	1.80	3 (13%)
55	4SU	2x	8	55	18,21,22	1.98	6 (33%)	26,30,33	1.49	4 (15%)
32	5MC	1a	1404	32	18,22,23	1.01	2 (11%)	26,32,35	1.12	2 (7%)
1	PSU	2A	1911	1	18,21,22	1.34	2 (11%)	22,30,33	1.94	4 (18%)
1	PSU	2A	1917	1	18,21,22	1.34	2 (11%)	22,30,33	1.92	3 (13%)
32	G7M	1a	527	32	20,26,27	1.18	2 (10%)	17,39,42	0.70	0
1	PSU	1A	1917	1	18,21,22	1.34	2 (11%)	22,30,33	1.91	3 (13%)
43	0TD	2l	92	43	7,9,10	4.79	1 (14%)	6,11,13	3.45	3 (50%)
1	OMU	2A	2552	58,1	19,22,23	1.24	2 (10%)	26,31,34	1.70	5 (19%)
32	5MC	2a	967	32	18,22,23	0.93	2 (11%)	26,32,35	1.13	3 (11%)
57	MIA	2y	37	57	18,24,32	1.14	2 (11%)	18,35,47	1.25	2 (11%)
55	8AN	1x	76	58,56,55	19,24,25	1.36	3 (15%)	13,35,38	1.88	2 (15%)
32	UR3	1a	1498	32	19,22,23	1.06	1 (5%)	26,32,35	1.46	3 (11%)
54	PSU	1w	32	54,58	18,21,22	1.34	2 (11%)	22,30,33	1.81	3 (13%)
1	OMC	1A	1920	1	19,22,23	0.86	0	26,31,34	0.85	0
43	0TD	1l	92	43	7,9,10	4.81	2 (28%)	6,11,13	9.04	2 (33%)
32	5MC	1a	967	32	18,22,23	0.93	2 (11%)	26,32,35	1.18	3 (11%)
1	2MA	2A	2503	58,1	17,25,26	1.11	2 (11%)	17,37,40	0.90	2 (11%)
32	MA6	2a	1519	32	19,26,27	0.79	0	18,38,41	1.73	3 (16%)
57	PSU	2y	55	57	18,21,22	1.37	2 (11%)	22,30,33	1.83	4 (18%)
54	PSU	1w	55	54	18,21,22	1.36	2 (11%)	22,30,33	1.83	3 (13%)
32	M2G	2a	966	32	20,27,28	1.44	3 (15%)	22,40,43	1.03	2 (9%)
57	G7M	2y	46	57	20,26,27	1.37	2 (10%)	17,39,42	0.72	1 (5%)
54	MIA	1w	37	54	24,31,32	2.08	3 (12%)	26,44,47	3.00	10 (38%)
32	5MC	2a	1404	32	18,22,23	0.97	2 (11%)	26,32,35	1.18	2 (7%)
54	PSU	1w	39	54	18,21,22	1.28	2 (11%)	22,30,33	1.87	3 (13%)

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
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
1	OMU	1A	2552	58,1	-	0/9/27/28	0/2/2/2
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
57	5MU	1y	54	57	-	0/7/25/26	0/2/2/2
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	58,1	-	0/7/25/26	0/2/2/2
57	PSU	1y	39	57	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
54	F3N	1w	76	54,1	-	0/15/37/38	0/4/4/4
57	G7M	1y	46	57	-	2/3/25/26	0/3/3/3
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
54	PSU	2w	32	54	-	2/7/25/26	0/2/2/2
54	MIA	2w	37	54	-	0/7/29/34	0/3/3/3
57	PSU	1y	32	57	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/7/29/30	0/3/3/3
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
57	PSU	1y	55	57	-	2/7/25/26	0/2/2/2
1	5MC	1A	1962	1	-	0/7/25/26	0/2/2/2
55	5MU	1x	54	55	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32	-	3/9/29/30	0/2/2/2
32	2MG	1a	1207	32	-	0/5/27/28	0/3/3/3
1	5MU	1A	1939	58,1	-	0/7/25/26	0/2/2/2
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	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
54	G7M	1w	46	54	-	1/3/25/26	0/3/3/3
32	G7M	2a	527	58,32	-	3/3/25/26	0/3/3/3
1	OMG	2A	2251	58,55,1	-	0/5/27/28	0/3/3/3
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
54	F3N	2w	76	54,1	-	2/15/37/38	0/4/4/4
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
57	PSU	2y	32	57	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	0/9/29/30	0/2/2/2
32	MA6	2a	1518	32	-	0/7/29/30	0/3/3/3
1	OMG	1A	2251	58,55,1	-	0/5/27/28	0/3/3/3
32	5MC	1a	1400	32	-	2/7/25/26	0/2/2/2
55	8AN	2x	76	59,58,56,55	-	3/3/25/26	0/3/3/3
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MU	1A	1915	1	-	1/7/25/26	0/2/2/2
54	G7M	2w	46	54	-	3/3/25/26	0/3/3/3
32	MA6	1a	1519	32	-	3/7/29/30	0/3/3/3
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
57	MIA	1y	37	57	-	0/3/25/34	0/3/3/3
32	2MG	2a	1207	32	-	0/5/27/28	0/3/3/3
57	5MU	2y	54	57	-	2/7/25/26	0/2/2/2
54	PSU	2w	39	54	-	1/7/25/26	0/2/2/2
57	PSU	2y	39	42,57	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
54	4SU	2w	8	54	-	2/7/25/26	0/2/2/2
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
1	2MA	1A	2503	58,1	-	2/3/25/26	0/3/3/3
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
57	4SU	2y	8	57	-	2/7/25/26	0/2/2/2
57	4SU	1y	8	57	-	2/7/25/26	0/2/2/2
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	1	-	0/7/25/26	0/2/2/2
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
32	PSU	1a	516	58,32	-	0/7/25/26	0/2/2/2
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
55	4SU	2x	8	55	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
32	G7M	1a	527	32	-	3/3/25/26	0/3/3/3
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	3/7/12/14	-
1	OMU	2A	2552	58,1	-	0/9/27/28	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
57	MIA	2y	37	57	-	2/3/25/34	0/3/3/3
55	8AN	1x	76	58,56,55	-	3/3/25/26	0/3/3/3
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
54	PSU	1w	32	54,58	-	0/7/25/26	0/2/2/2
1	OMC	1A	1920	1	-	1/9/27/28	0/2/2/2
43	0TD	1l	92	43	-	2/7/12/14	-
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	58,1	-	2/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	MA6	2a	1519	32	-	3/7/29/30	0/3/3/3
57	PSU	2y	55	57	-	1/7/25/26	0/2/2/2
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
57	G7M	2y	46	57	-	0/3/25/26	0/3/3/3
54	MIA	1w	37	54	-	3/11/33/34	0/3/3/3
32	5MC	2a	1404	32	-	1/7/25/26	0/2/2/2
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2

All (205) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.36	1.69	1.82
43	1l	92	0TD	CB-SB	-12.23	1.69	1.82
54	2w	37	MIA	C2-S10	-7.29	1.69	1.75
54	1w	37	MIA	C13-C14	6.89	1.52	1.32
54	1w	37	MIA	C2-S10	-6.17	1.70	1.75
54	2w	76	F3N	CB-CG	-4.76	1.39	1.51
55	1x	8	4SU	C4-N3	-4.66	1.32	1.37
32	2a	966	M2G	C2-N3	4.65	1.36	1.30
54	2w	8	4SU	C4-S4	-4.61	1.59	1.68
54	1w	76	F3N	CB-CG	-4.53	1.40	1.51
55	2x	8	4SU	C4-N3	-4.49	1.32	1.37
32	1a	966	M2G	C2-N3	4.46	1.36	1.30
54	1w	8	4SU	C4-S4	-4.38	1.60	1.68
57	2y	8	4SU	C4-S4	-4.26	1.60	1.68
55	2x	8	4SU	C4-S4	-4.20	1.60	1.68
57	2y	46	G7M	C5-C4	4.16	1.47	1.39
57	1y	46	G7M	C5-C4	4.15	1.47	1.39
57	1y	8	4SU	C4-S4	-4.06	1.60	1.68
54	1w	8	4SU	C4-N3	-4.04	1.33	1.37
54	2w	39	PSU	C6-C5	3.98	1.40	1.35
57	2y	39	PSU	C6-C5	3.96	1.39	1.35
55	1x	8	4SU	C4-S4	-3.91	1.61	1.68
54	1w	55	PSU	C6-C5	3.90	1.39	1.35
32	1a	527	G7M	C5-C4	3.82	1.46	1.39
57	1y	32	PSU	C6-C5	3.79	1.39	1.35
57	1y	39	PSU	C6-C5	3.78	1.39	1.35
54	2w	46	G7M	C5-C4	3.76	1.46	1.39
54	2w	55	PSU	C6-C5	3.76	1.39	1.35
57	1y	55	PSU	C6-C5	3.72	1.39	1.35
55	1x	8	4SU	C2-N3	-3.70	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	46	G7M	C5-C4	3.68	1.46	1.39
32	2a	516	PSU	C6-C5	3.68	1.39	1.35
57	2y	32	PSU	C6-C5	3.64	1.39	1.35
54	2w	32	PSU	C6-C5	3.62	1.39	1.35
55	1x	55	PSU	C6-C5	3.50	1.39	1.35
32	2a	527	G7M	C5-C4	3.50	1.46	1.39
1	2A	1917	PSU	C6-C5	3.34	1.39	1.35
1	1A	1917	PSU	C6-C5	3.31	1.39	1.35
32	1a	516	PSU	C6-C5	3.30	1.39	1.35
55	2x	55	PSU	C6-C5	3.29	1.39	1.35
54	1w	32	PSU	C6-C5	3.28	1.39	1.35
55	1x	8	4SU	C5-C4	-3.26	1.38	1.42
57	2y	55	PSU	C6-C5	3.23	1.39	1.35
1	2A	1911	PSU	C6-C5	3.20	1.39	1.35
1	1A	2605	PSU	C4-N3	-3.19	1.32	1.38
54	1w	39	PSU	C6-C5	3.16	1.39	1.35
57	2y	54	5MU	C6-C5	3.14	1.39	1.34
57	2y	54	5MU	C2-N1	3.09	1.43	1.38
55	2x	8	4SU	C5-C4	-3.04	1.38	1.42
1	1A	1911	PSU	C6-C5	3.04	1.38	1.35
54	2w	76	F3N	O4'-C1'	3.03	1.45	1.41
1	2A	2605	PSU	C6-C5	3.01	1.38	1.35
1	2A	1939	5MU	C6-C5	2.99	1.39	1.34
54	1w	76	F3N	O4'-C1'	2.98	1.45	1.41
57	2y	8	4SU	C4-N3	-2.98	1.34	1.37
1	2A	1942	5MC	C6-C5	2.94	1.39	1.34
1	2A	1962	5MC	C6-C5	2.94	1.39	1.34
54	2w	54	5MU	C6-C5	2.93	1.39	1.34
1	1A	2605	PSU	C6-C5	2.91	1.38	1.35
55	1x	54	5MU	C4-N3	-2.89	1.33	1.38
32	1a	1400	5MC	C6-C5	2.89	1.39	1.34
32	1a	966	M2G	C2-N2	2.88	1.40	1.35
1	2A	1915	5MU	C6-C5	2.86	1.39	1.34
54	2w	8	4SU	C4-N3	-2.85	1.34	1.37
32	2a	1400	5MC	C6-C5	2.84	1.39	1.34
57	1y	54	5MU	C6-C5	2.83	1.39	1.34
32	1a	1407	5MC	C6-C5	2.83	1.39	1.34
55	1x	76	8AN	C5-C4	-2.81	1.33	1.40
54	1w	76	F3N	C5-C4	-2.81	1.33	1.40
55	2x	76	8AN	C5-C4	-2.80	1.33	1.40
1	2A	1915	5MU	C4-C5	2.80	1.49	1.44
32	2a	1404	5MC	C6-C5	2.79	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1962	5MC	C6-C5	2.79	1.39	1.34
57	2y	37	MIA	C2-N3	2.78	1.36	1.32
57	2y	37	MIA	C5-C4	2.78	1.48	1.40
55	1x	54	5MU	C6-C5	2.78	1.39	1.34
54	2w	76	F3N	C5-C4	-2.77	1.33	1.40
55	2x	8	4SU	C2-N3	-2.76	1.33	1.38
57	1y	8	4SU	C4-N3	-2.76	1.34	1.37
54	1w	32	PSU	C4-N3	-2.75	1.33	1.38
32	2a	966	M2G	C2-N2	2.73	1.40	1.35
57	1y	8	4SU	C2-N1	2.73	1.42	1.38
54	1w	37	MIA	C5-C4	2.72	1.48	1.40
1	2A	1915	5MU	C2-N1	2.72	1.42	1.38
1	1A	1939	5MU	C4-C5	2.72	1.49	1.44
1	1A	1942	5MC	C6-C5	2.71	1.39	1.34
54	2w	37	MIA	C5-C4	2.69	1.48	1.40
57	1y	37	MIA	C5-C4	2.69	1.48	1.40
57	2y	54	5MU	C4-N3	-2.67	1.33	1.38
55	2x	54	5MU	C6-C5	2.66	1.39	1.34
57	1y	37	MIA	C2-N3	2.66	1.36	1.32
54	1w	8	4SU	C5-C4	-2.64	1.39	1.42
57	2y	8	4SU	C2-N1	2.63	1.42	1.38
1	2A	2503	2MA	C2-N3	2.63	1.36	1.31
55	2x	76	8AN	C6-C5	-2.62	1.33	1.43
57	1y	54	5MU	C4-C5	2.62	1.49	1.44
54	1w	54	5MU	C6-C5	2.62	1.38	1.34
32	1a	1404	5MC	C6-C5	2.62	1.38	1.34
1	1A	1911	PSU	C4-N3	-2.61	1.34	1.38
1	1A	1939	5MU	C4-N3	-2.60	1.34	1.38
1	2A	1911	PSU	C4-N3	-2.60	1.34	1.38
1	1A	1939	5MU	C6-N1	-2.60	1.33	1.38
32	1a	516	PSU	C4-N3	-2.60	1.34	1.38
1	1A	2552	OMU	C4-N3	-2.58	1.33	1.38
55	2x	54	5MU	C4-N3	-2.58	1.34	1.38
32	1a	1207	2MG	C6-N1	-2.57	1.34	1.37
1	1A	1939	5MU	C6-C5	2.56	1.38	1.34
1	2A	1917	PSU	C4-N3	-2.55	1.34	1.38
32	2a	967	5MC	C6-C5	2.55	1.38	1.34
57	2y	55	PSU	C4-N3	-2.54	1.34	1.38
55	1x	32	5MC	C6-C5	2.53	1.38	1.34
1	1A	1939	5MU	C2-N3	-2.53	1.33	1.38
55	1x	76	8AN	C6-C5	-2.52	1.33	1.43
1	2A	2552	OMU	C4-N3	-2.51	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2w	76	F3N	C6-C5	-2.51	1.34	1.43
1	2A	2251	OMG	C6-N1	-2.50	1.34	1.37
55	2x	55	PSU	C4-N3	-2.49	1.34	1.38
1	2A	1939	5MU	C4-N3	-2.48	1.34	1.38
54	1w	8	4SU	C2-N3	-2.48	1.33	1.38
32	1a	967	5MC	C6-C5	2.48	1.38	1.34
55	1x	8	4SU	O2-C2	2.48	1.27	1.23
32	1a	966	M2G	C6-N1	-2.47	1.34	1.37
54	1w	76	F3N	C6-C5	-2.47	1.34	1.43
1	1A	1917	PSU	C4-N3	-2.46	1.34	1.38
55	1x	55	PSU	C4-N3	-2.45	1.34	1.38
54	1w	54	5MU	C2-N1	2.45	1.42	1.38
55	2x	32	5MC	C6-C5	2.45	1.38	1.34
32	1a	1498	UR3	C2-N1	2.45	1.42	1.38
1	2A	2552	OMU	C5-C4	2.45	1.49	1.43
55	2x	54	5MU	C4-C5	2.44	1.48	1.44
54	2w	32	PSU	C4-N3	-2.44	1.34	1.38
54	2w	8	4SU	C5-C4	-2.43	1.39	1.42
32	2a	1207	2MG	C6-N1	-2.41	1.34	1.37
32	2a	1407	5MC	C6-N1	-2.41	1.33	1.38
55	1x	32	5MC	C6-N1	-2.41	1.33	1.38
54	1w	39	PSU	C4-N3	-2.41	1.34	1.38
32	2a	1400	5MC	C6-N1	-2.40	1.33	1.38
55	2x	54	5MU	C2-N1	2.40	1.42	1.38
57	1y	8	4SU	C5-C4	-2.39	1.39	1.42
57	1y	54	5MU	C4-N3	-2.39	1.34	1.38
1	2A	1962	5MC	C6-N1	-2.39	1.34	1.38
57	1y	39	PSU	C4-N3	-2.39	1.34	1.38
1	2A	1939	5MU	C2-N1	2.38	1.42	1.38
55	2x	32	5MC	C6-N1	-2.37	1.34	1.38
32	2a	1407	5MC	C6-C5	2.37	1.38	1.34
54	2w	54	5MU	C4-N3	-2.36	1.34	1.38
32	2a	527	G7M	C6-N1	-2.35	1.34	1.37
1	2A	1915	5MU	C4-N3	-2.35	1.34	1.38
32	1a	967	5MC	C6-N1	-2.34	1.34	1.38
1	1A	1915	5MU	C6-C5	2.33	1.38	1.34
1	1A	1915	5MU	C4-N3	-2.32	1.34	1.38
1	1A	1915	5MU	C4-C5	2.31	1.48	1.44
32	2a	966	M2G	C6-N1	-2.30	1.34	1.37
32	1a	1404	5MC	C6-N1	-2.30	1.34	1.38
57	2y	32	PSU	C4-N3	-2.29	1.34	1.38
55	2x	8	4SU	O2-C2	2.29	1.27	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	1y	54	5MU	C2-N1	2.29	1.42	1.38
57	1y	32	PSU	C4-N3	-2.29	1.34	1.38
1	1A	1962	5MC	C6-N1	-2.28	1.34	1.38
1	1A	1915	5MU	C2-N1	2.28	1.42	1.38
32	2a	1404	5MC	C6-N1	-2.28	1.34	1.38
1	2A	1939	5MU	C4-C5	2.27	1.48	1.44
54	2w	55	PSU	C4-N3	-2.27	1.34	1.38
54	2w	54	5MU	C2-N1	2.27	1.42	1.38
57	2y	54	5MU	C2-N3	-2.25	1.34	1.38
1	1A	2503	2MA	C2-N3	2.25	1.36	1.31
32	1a	1400	5MC	C6-N1	-2.25	1.34	1.38
54	1w	55	PSU	C4-N3	-2.24	1.34	1.38
57	1y	55	PSU	C4-N3	-2.23	1.34	1.38
57	2y	46	G7M	C6-N1	-2.23	1.34	1.37
57	2y	8	4SU	C5-C4	-2.23	1.39	1.42
57	2y	39	PSU	C4-N3	-2.22	1.34	1.38
1	1A	1939	5MU	C2-N1	2.22	1.42	1.38
55	1x	54	5MU	C2-N3	-2.18	1.34	1.38
54	2w	54	5MU	C4-C5	2.16	1.48	1.44
54	1w	8	4SU	C2-N1	2.16	1.41	1.38
1	2A	1915	5MU	C6-N1	-2.15	1.34	1.38
54	2w	39	PSU	C4-N3	-2.15	1.34	1.38
1	1A	2552	OMU	C5-C4	2.14	1.48	1.43
1	1A	1915	5MU	C6-N1	-2.14	1.34	1.38
54	2w	76	F3N	C5-N7	-2.14	1.32	1.39
32	2a	967	5MC	C6-N1	-2.14	1.34	1.38
57	2y	54	5MU	O2-C2	2.13	1.26	1.23
32	2a	516	PSU	C4-N3	-2.13	1.34	1.38
54	1w	54	5MU	C4-N3	-2.13	1.34	1.38
32	1a	527	G7M	C6-N1	-2.12	1.34	1.37
1	1A	1942	5MC	C6-N1	-2.12	1.34	1.38
55	2x	54	5MU	C6-N1	-2.12	1.34	1.38
55	1x	54	5MU	C6-N1	-2.11	1.34	1.38
55	2x	76	8AN	C5-N7	-2.11	1.32	1.39
57	1y	46	G7M	C6-N1	-2.10	1.34	1.37
55	1x	76	8AN	C5-N7	-2.10	1.32	1.39
1	1A	2251	OMG	C6-N1	-2.10	1.34	1.37
1	2A	2605	PSU	C4-N3	-2.08	1.35	1.38
54	1w	76	F3N	C5-N7	-2.08	1.32	1.39
55	2x	8	4SU	C2-N1	2.07	1.41	1.38
43	1l	92	0TD	CB-CG	2.07	1.55	1.52
1	2A	1939	5MU	C2-N3	-2.06	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2605	PSU	C2-N3	-2.06	1.34	1.37
1	2A	1939	5MU	C6-N1	-2.05	1.34	1.38
1	2A	2605	PSU	C2-N1	-2.05	1.34	1.36
55	1x	54	5MU	C2-N1	2.04	1.41	1.38
54	1w	46	G7M	C6-N1	-2.04	1.34	1.37
1	2A	2503	2MA	C6-N1	-2.03	1.33	1.38
1	1A	2503	2MA	C6-N6	2.01	1.36	1.28

All (286) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	1l	92	0TD	CSB-SB-CB	-21.73	63.14	102.44
54	1w	37	MIA	C12-C13-C14	-9.67	108.32	127.14
54	2w	8	4SU	C4-N3-C2	-7.62	119.94	127.34
43	2l	92	0TD	CSB-SB-CB	-7.22	89.37	102.44
54	2w	8	4SU	C5-C4-N3	6.58	120.79	114.69
1	1A	2605	PSU	N1-C2-N3	6.27	122.24	115.13
54	1w	37	MIA	C12-N6-C6	-6.14	113.46	122.55
1	2A	1917	PSU	N1-C2-N3	6.08	122.02	115.13
1	1A	1911	PSU	N1-C2-N3	6.04	121.97	115.13
32	2a	1498	UR3	C4-N3-C2	-6.03	118.89	124.56
57	2y	8	4SU	C4-N3-C2	-5.97	121.54	127.34
55	2x	54	5MU	C4-N3-C2	-5.97	119.62	127.35
55	2x	55	PSU	N1-C2-N3	5.92	121.84	115.13
57	1y	55	PSU	N1-C2-N3	5.89	121.81	115.13
1	2A	1911	PSU	N1-C2-N3	5.88	121.79	115.13
1	2A	2605	PSU	N1-C2-N3	5.85	121.76	115.13
57	2y	32	PSU	N1-C2-N3	5.81	121.71	115.13
54	1w	32	PSU	N1-C2-N3	5.75	121.65	115.13
1	1A	1917	PSU	N1-C2-N3	5.73	121.62	115.13
54	1w	39	PSU	N1-C2-N3	5.69	121.57	115.13
32	1a	1498	UR3	C4-N3-C2	-5.68	119.21	124.56
32	1a	516	PSU	N1-C2-N3	5.65	121.53	115.13
55	1x	76	8AN	N3-C2-N1	-5.64	119.87	128.68
57	1y	39	PSU	N1-C2-N3	5.63	121.51	115.13
32	2a	516	PSU	N1-C2-N3	5.60	121.48	115.13
54	1w	76	F3N	N3-C2-N1	-5.60	119.93	128.68
57	1y	8	4SU	C4-N3-C2	-5.58	121.92	127.34
1	1A	1939	5MU	C5-C4-N3	5.56	120.06	115.31
54	2w	55	PSU	N1-C2-N3	5.56	121.43	115.13
54	1w	55	PSU	N1-C2-N3	5.55	121.42	115.13
54	2w	76	F3N	N3-C2-N1	-5.55	120.01	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	2x	76	8AN	N3-C2-N1	-5.54	120.02	128.68
57	2y	8	4SU	C5-C4-N3	5.52	119.81	114.69
55	1x	55	PSU	N1-C2-N3	5.51	121.38	115.13
55	2x	54	5MU	N3-C2-N1	5.49	122.18	114.89
1	1A	1939	5MU	C4-N3-C2	-5.40	120.37	127.35
57	2y	55	PSU	N1-C2-N3	5.37	121.21	115.13
57	1y	32	PSU	N1-C2-N3	5.35	121.19	115.13
54	2w	32	PSU	N1-C2-N3	5.35	121.19	115.13
54	1w	54	5MU	C4-N3-C2	-5.26	120.54	127.35
1	1A	2552	OMU	N3-C2-N1	5.26	121.87	114.89
57	2y	39	PSU	N1-C2-N3	5.25	121.08	115.13
32	2a	1519	MA6	N3-C2-N1	-5.22	120.52	128.68
54	1w	54	5MU	O4-C4-C5	-5.15	118.93	124.90
1	1A	1915	5MU	C4-N3-C2	-5.14	120.70	127.35
54	1w	8	4SU	C5-C4-N3	5.09	119.41	114.69
1	2A	1939	5MU	C4-N3-C2	-5.07	120.79	127.35
55	2x	54	5MU	C5-C4-N3	5.07	119.64	115.31
32	1a	1518	MA6	N3-C2-N1	-5.07	120.76	128.68
32	2a	1518	MA6	N3-C2-N1	-5.07	120.76	128.68
54	2w	39	PSU	N1-C2-N3	5.06	120.87	115.13
1	2A	1915	5MU	C4-N3-C2	-5.06	120.81	127.35
57	1y	8	4SU	C5-C4-N3	5.04	119.37	114.69
32	1a	1519	MA6	N3-C2-N1	-4.89	121.04	128.68
1	2A	2552	OMU	N3-C2-N1	4.86	121.34	114.89
54	1w	54	5MU	N3-C2-N1	4.85	121.33	114.89
1	2A	1915	5MU	N3-C2-N1	4.80	121.26	114.89
54	1w	54	5MU	C5-C4-N3	4.77	119.38	115.31
1	2A	1939	5MU	N3-C2-N1	4.77	121.22	114.89
1	2A	1939	5MU	C5-C4-N3	4.74	119.36	115.31
55	1x	8	4SU	O2-C2-N1	4.68	129.01	122.79
1	1A	1915	5MU	C5-C4-N3	4.66	119.29	115.31
1	1A	1915	5MU	N3-C2-N1	4.63	121.03	114.89
55	1x	54	5MU	C4-N3-C2	-4.61	121.38	127.35
1	1A	1915	5MU	O4-C4-C5	-4.59	119.58	124.90
57	1y	54	5MU	C4-N3-C2	-4.52	121.50	127.35
54	1w	37	MIA	C15-C14-C13	-4.48	109.69	122.65
1	1A	2605	PSU	C4-N3-C2	-4.46	119.91	126.34
55	1x	54	5MU	N3-C2-N1	4.45	120.79	114.89
1	1A	1939	5MU	C5-C6-N1	-4.43	118.78	123.34
57	1y	54	5MU	N3-C2-N1	4.42	120.75	114.89
1	2A	1915	5MU	C5-C4-N3	4.41	119.08	115.31
1	2A	2605	PSU	C4-N3-C2	-4.41	119.99	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	1x	54	5MU	C5-C4-N3	4.33	119.01	115.31
1	2A	1939	5MU	O4-C4-C5	-4.30	119.92	124.90
54	2w	8	4SU	C5-C4-S4	-4.29	118.94	124.47
1	2A	1911	PSU	C4-N3-C2	-4.25	120.22	126.34
54	1w	37	MIA	C2-N3-C4	4.23	121.15	115.32
54	2w	8	4SU	N3-C2-N1	4.22	120.49	114.89
1	1A	1939	5MU	N3-C2-N1	4.22	120.49	114.89
54	2w	37	MIA	C12-N6-C6	-4.20	119.26	122.87
54	2w	54	5MU	N3-C2-N1	4.19	120.46	114.89
54	1w	39	PSU	C4-N3-C2	-4.18	120.31	126.34
57	1y	54	5MU	C5-C4-N3	4.18	118.88	115.31
1	2A	2552	OMU	C4-N3-C2	-4.17	121.08	126.58
55	2x	54	5MU	O4-C4-C5	-4.14	120.10	124.90
1	2A	2605	PSU	O2-C2-N1	-4.13	118.24	122.79
54	2w	54	5MU	O4-C4-C5	-4.11	120.14	124.90
1	1A	1911	PSU	C4-N3-C2	-4.10	120.43	126.34
1	1A	1917	PSU	O2-C2-N1	-4.05	118.33	122.79
32	2a	1404	5MC	C5-C6-N1	-4.05	119.18	123.34
55	1x	8	4SU	C6-C5-C4	-4.04	116.46	119.95
54	2w	54	5MU	C4-N3-C2	-4.04	122.13	127.35
55	2x	32	5MC	C5-C6-N1	-3.99	119.23	123.34
54	2w	37	MIA	C2-N3-C4	3.95	120.77	115.32
1	2A	1917	PSU	C4-N3-C2	-3.95	120.64	126.34
57	1y	8	4SU	C1'-N1-C2	3.93	124.69	117.57
55	2x	55	PSU	C4-N3-C2	-3.93	120.67	126.34
55	1x	54	5MU	O4-C4-C5	-3.93	120.35	124.90
57	1y	39	PSU	C4-N3-C2	-3.93	120.68	126.34
1	1A	1911	PSU	O2-C2-N1	-3.92	118.47	122.79
55	2x	8	4SU	C5-C4-N3	3.89	118.30	114.69
1	1A	1917	PSU	C4-N3-C2	-3.88	120.75	126.34
54	1w	55	PSU	O2-C2-N1	-3.88	118.52	122.79
57	1y	55	PSU	O2-C2-N1	-3.86	118.54	122.79
54	2w	54	5MU	C5-C4-N3	3.84	118.59	115.31
32	2a	1400	5MC	C5-C6-N1	-3.83	119.40	123.34
55	1x	54	5MU	C5-C6-N1	-3.82	119.41	123.34
57	2y	54	5MU	O4-C4-C5	-3.81	120.49	124.90
32	2a	1407	5MC	C5-C6-N1	-3.81	119.42	123.34
32	2a	516	PSU	C4-N3-C2	-3.80	120.86	126.34
54	1w	37	MIA	C16-C14-C13	-3.80	111.67	122.65
57	2y	32	PSU	C4-N3-C2	-3.77	120.90	126.34
57	2y	54	5MU	C5-C4-N3	3.76	118.52	115.31
1	2A	1917	PSU	O2-C2-N1	-3.75	118.66	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	1942	5MC	C5-C6-N1	-3.75	119.48	123.34
55	2x	54	5MU	C5-C6-N1	-3.74	119.49	123.34
1	2A	1962	5MC	C5-C6-N1	-3.73	119.50	123.34
57	2y	8	4SU	N3-C2-N1	3.67	119.77	114.89
54	1w	32	PSU	C4-N3-C2	-3.67	121.06	126.34
57	1y	32	PSU	O2-C2-N1	-3.66	118.76	122.79
32	1a	516	PSU	C4-N3-C2	-3.64	121.09	126.34
1	2A	1911	PSU	O2-C2-N1	-3.64	118.78	122.79
57	1y	8	4SU	N3-C2-N1	3.63	119.71	114.89
1	1A	2552	OMU	O2-C2-N1	-3.63	117.96	122.79
1	2A	1939	5MU	C5-C6-N1	-3.61	119.63	123.34
57	1y	8	4SU	C5-C4-S4	-3.59	119.84	124.47
1	2A	2552	OMU	O2-C2-N1	-3.57	118.03	122.79
55	1x	8	4SU	C1'-N1-C2	3.56	124.02	117.57
1	2A	1942	5MC	C5-C6-N1	-3.56	119.68	123.34
54	1w	8	4SU	C4-N3-C2	-3.56	123.88	127.34
57	2y	55	PSU	C4-N3-C2	-3.56	121.22	126.34
32	1a	967	5MC	C5-C6-N1	-3.55	119.69	123.34
55	1x	32	5MC	C5-C6-N1	-3.55	119.69	123.34
32	1a	1400	5MC	C5-C6-N1	-3.54	119.70	123.34
57	1y	54	5MU	O4-C4-C5	-3.53	120.81	124.90
55	1x	55	PSU	C4-N3-C2	-3.48	121.32	126.34
57	1y	37	MIA	N3-C2-N1	-3.48	123.25	128.68
54	2w	37	MIA	C11-S10-C2	-3.47	99.67	102.27
54	2w	37	MIA	C5-C6-N1	-3.47	117.93	120.81
1	2A	1915	5MU	O4-C4-C5	-3.46	120.89	124.90
1	1A	2552	OMU	C4-N3-C2	-3.46	122.02	126.58
54	2w	55	PSU	C4-N3-C2	-3.44	121.39	126.34
54	2w	55	PSU	O2-C2-N1	-3.43	119.02	122.79
54	2w	32	PSU	C4-N3-C2	-3.42	121.41	126.34
1	2A	1915	5MU	C5-C6-N1	-3.41	119.83	123.34
57	1y	32	PSU	C4-N3-C2	-3.39	121.45	126.34
1	1A	1939	5MU	O4-C4-C5	-3.39	120.97	124.90
32	2a	516	PSU	O2-C2-N1	-3.37	119.08	122.79
57	1y	55	PSU	C4-N3-C2	-3.35	121.51	126.34
32	1a	1519	MA6	C4-C5-N7	-3.33	105.93	109.40
55	2x	8	4SU	C1'-N1-C2	3.31	123.57	117.57
32	2a	1519	MA6	C4-C5-N7	-3.29	105.97	109.40
43	2l	92	0TD	OD2-CG-CB	3.29	120.25	113.15
54	1w	37	MIA	C2-N1-C6	3.28	123.06	117.19
57	2y	39	PSU	C4-N3-C2	-3.28	121.61	126.34
43	1l	92	0TD	OD2-CG-CB	3.28	120.23	113.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	967	5MC	C5-C6-N1	-3.28	119.97	123.34
54	2w	39	PSU	C4-N3-C2	-3.27	121.63	126.34
54	1w	37	MIA	C5-C6-N1	-3.27	118.10	120.81
32	1a	1407	5MC	C5-C6-N1	-3.26	119.98	123.34
55	1x	8	4SU	C5-C4-N3	3.26	117.72	114.69
1	1A	1962	5MC	C5-C6-N1	-3.25	119.99	123.34
55	2x	55	PSU	O2-C2-N1	-3.25	119.22	122.79
55	2x	8	4SU	C6-C5-C4	-3.24	117.14	119.95
57	2y	32	PSU	O2-C2-N1	-3.20	119.27	122.79
54	1w	55	PSU	C4-N3-C2	-3.19	121.74	126.34
32	1a	1404	5MC	C5-C6-N1	-3.18	120.07	123.34
57	2y	37	MIA	N3-C2-N1	-3.18	123.71	128.68
57	2y	55	PSU	O2-C2-N1	-3.16	119.31	122.79
57	2y	8	4SU	C5-C4-S4	-3.14	120.42	124.47
57	2y	55	PSU	C6-C5-C4	-3.11	116.03	118.20
55	2x	76	8AN	O4'-C1'-C2'	-3.07	102.43	106.93
57	2y	54	5MU	N3-C2-N1	3.05	118.94	114.89
55	1x	55	PSU	O2-C2-N1	-3.03	119.46	122.79
54	1w	39	PSU	O2-C2-N1	-3.03	119.46	122.79
57	1y	54	5MU	C5-C6-N1	-3.01	120.24	123.34
55	2x	54	5MU	O2-C2-N1	-2.98	118.82	122.79
32	2a	1518	MA6	C4-C5-N7	-2.97	106.31	109.40
1	2A	2251	OMG	C5-C6-N1	2.96	119.19	113.95
32	1a	1404	5MC	C5-C4-N3	-2.95	118.49	121.67
54	2w	39	PSU	O2-C2-N1	-2.94	119.56	122.79
54	1w	54	5MU	C5-C6-N1	-2.92	120.34	123.34
1	1A	1915	5MU	C5-C6-N1	-2.90	120.36	123.34
57	2y	37	MIA	C4-C5-N7	-2.88	106.40	109.40
32	2a	1402	4OC	CM4-N4-C4	-2.87	116.84	122.45
55	1x	32	5MC	C5-C4-N3	-2.82	118.63	121.67
1	1A	1939	5MU	C5M-C5-C4	2.79	121.84	118.77
54	2w	39	PSU	C6-C5-C4	-2.79	116.25	118.20
32	1a	1518	MA6	C4-C5-N7	-2.79	106.49	109.40
57	2y	39	PSU	O2-C2-N1	-2.79	119.72	122.79
54	2w	32	PSU	O2-C2-N1	-2.76	119.75	122.79
54	2w	37	MIA	C4-C5-N7	-2.76	106.53	109.40
54	1w	37	MIA	C11-S10-C2	-2.75	100.21	102.27
54	2w	8	4SU	O2-C2-N1	-2.73	119.15	122.79
57	2y	54	5MU	C4-N3-C2	-2.73	123.82	127.35
57	2y	54	5MU	C1'-N1-C2	2.73	122.50	117.57
55	1x	8	4SU	O2-C2-N3	-2.71	116.46	121.50
32	1a	1207	2MG	C8-N7-C5	2.70	108.13	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	1519	MA6	C1'-N9-C4	-2.68	121.92	126.64
32	2a	1402	4OC	O2-C2-N3	-2.66	118.01	122.33
54	1w	37	MIA	C4-C5-N7	-2.63	106.66	109.40
1	2A	1942	5MC	C5-C4-N3	-2.62	118.84	121.67
1	2A	1915	5MU	C5M-C5-C4	2.62	121.65	118.77
1	1A	1915	5MU	C5M-C5-C4	2.62	121.65	118.77
1	1A	1915	5MU	O2-C2-N1	-2.61	119.31	122.79
43	2l	92	0TD	OD1-CG-CB	-2.60	116.99	122.44
54	2w	54	5MU	C5-C6-N1	-2.60	120.67	123.34
57	1y	39	PSU	O2-C2-N1	-2.58	119.94	122.79
32	2a	1407	5MC	C5-C4-N3	-2.58	118.89	121.67
32	1a	516	PSU	O2-C2-N1	-2.58	119.95	122.79
54	1w	37	MIA	N3-C2-N1	-2.58	122.23	126.98
54	1w	32	PSU	O2-C2-N1	-2.57	119.96	122.79
55	1x	76	8AN	O4'-C1'-C2'	-2.57	103.17	106.93
57	2y	8	4SU	C1'-N1-C2	2.57	122.22	117.57
1	2A	1962	5MC	C5-C4-N3	-2.56	118.91	121.67
32	1a	1400	5MC	C5-C4-N3	-2.56	118.92	121.67
55	2x	32	5MC	C5-C4-N3	-2.54	118.93	121.67
32	2a	1400	5MC	C5-C4-N3	-2.54	118.93	121.67
1	1A	1962	5MC	C5-C4-N3	-2.53	118.94	121.67
32	1a	966	M2G	C8-N7-C5	2.52	107.80	102.99
32	1a	1498	UR3	C1'-N1-C2	2.51	121.23	116.99
32	2a	1404	5MC	C5-C4-N3	-2.48	119.00	121.67
1	2A	2552	OMU	C5-C4-N3	2.48	118.55	114.84
55	2x	32	5MC	CM5-C5-C6	-2.47	119.54	122.85
1	2A	2503	2MA	C8-N7-C5	2.47	107.69	102.99
1	2A	2552	OMU	O4-C4-C5	-2.46	120.83	125.16
57	2y	54	5MU	O2-C2-N3	-2.46	116.93	121.50
54	2w	32	PSU	C6-C5-C4	-2.45	116.48	118.20
1	1A	2605	PSU	C5-C6-N1	-2.45	118.44	122.11
57	1y	37	MIA	C4-C5-N7	-2.45	106.85	109.40
1	1A	1942	5MC	C5-C4-N3	-2.44	119.05	121.67
54	1w	54	5MU	O2-C2-N1	-2.43	119.55	122.79
54	1w	8	4SU	N3-C2-N1	2.42	118.11	114.89
54	2w	37	MIA	C2-N1-C6	2.42	121.52	117.19
1	1A	2605	PSU	O2-C2-N3	-2.41	117.27	121.82
32	2a	966	M2G	C8-N7-C5	2.41	107.58	102.99
32	1a	1407	5MC	C5-C4-N3	-2.40	119.09	121.67
55	1x	8	4SU	S4-C4-N3	-2.39	117.85	120.21
1	1A	2251	OMG	C5-C6-N1	2.38	118.16	113.95
1	2A	2251	OMG	O6-C6-C5	-2.38	119.72	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	2x	32	5MC	O2-C2-N3	-2.38	118.47	122.33
32	2a	1207	2MG	C8-N7-C5	2.37	107.50	102.99
32	1a	1402	4OC	C6-C5-C4	2.36	119.85	116.96
32	1a	966	M2G	C5-C6-N1	2.36	118.11	113.95
54	1w	8	4SU	C1'-N1-C2	2.33	121.79	117.57
57	2y	54	5MU	C1'-N1-C6	-2.32	117.26	121.12
32	1a	967	5MC	CM5-C5-C6	-2.32	119.76	122.85
57	2y	54	5MU	C5-C6-N1	-2.31	120.96	123.34
57	1y	32	PSU	C6-C5-C4	-2.30	116.59	118.20
1	1A	2251	OMG	O6-C6-C5	-2.30	119.89	124.37
1	1A	2251	OMG	C8-N7-C5	2.29	107.36	102.99
32	1a	1407	5MC	O2-C2-N3	-2.29	118.61	122.33
32	1a	1498	UR3	C3U-N3-C2	2.28	121.31	117.31
55	2x	76	8AN	O2'-C2'-C3'	2.27	117.39	111.47
32	1a	1400	5MC	O2-C2-N3	-2.26	118.66	122.33
32	2a	966	M2G	C5-C6-N1	2.25	117.93	113.95
32	2a	1207	2MG	CM2-N2-C2	-2.25	118.90	123.86
1	1A	2552	OMU	O4-C4-C5	-2.22	121.25	125.16
1	1A	2503	2MA	C8-N7-C5	2.22	107.23	102.99
55	2x	32	5MC	C1'-N1-C6	-2.22	117.42	121.12
1	2A	1911	PSU	C5-C6-N1	-2.21	118.80	122.11
32	2a	967	5MC	CM5-C5-C6	-2.21	119.90	122.85
32	2a	1402	4OC	C6-C5-C4	2.20	119.66	116.96
32	2a	967	5MC	C5-C4-N3	-2.19	119.31	121.67
57	1y	54	5MU	C5M-C5-C4	2.18	121.17	118.77
32	1a	516	PSU	O4'-C1'-C2'	2.18	108.21	105.14
55	2x	8	4SU	O2-C2-N1	2.17	125.67	122.79
1	2A	1915	5MU	C5M-C5-C6	-2.17	119.96	122.85
1	2A	2251	OMG	C8-N7-C5	2.14	107.06	102.99
1	2A	2251	OMG	C2-N1-C6	-2.13	121.17	125.10
32	1a	1207	2MG	C5-C6-N1	2.10	117.67	113.95
1	1A	2605	PSU	O2-C2-N1	-2.09	120.49	122.79
57	1y	55	PSU	O4'-C1'-C2'	2.08	108.08	105.14
57	2y	39	PSU	C6-C5-C4	-2.07	116.75	118.20
32	2a	516	PSU	C6-C5-C4	-2.07	116.75	118.20
57	2y	32	PSU	O4'-C1'-C2'	2.07	108.07	105.14
57	1y	39	PSU	C6-C5-C4	-2.06	116.76	118.20
1	2A	2503	2MA	C5-C6-N1	2.05	117.56	114.02
1	2A	1939	5MU	O2-C2-N1	-2.04	120.08	122.79
32	2a	1407	5MC	CM5-C5-C6	-2.03	120.13	122.85
1	1A	1911	PSU	O4'-C1'-C2'	2.03	108.01	105.14
54	1w	8	4SU	C6-C5-C4	-2.03	118.20	119.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	2y	46	G7M	C3'-C2'-C1'	2.02	104.02	100.98
55	1x	54	5MU	O2-C2-N1	-2.01	120.11	122.79
32	1a	967	5MC	C5-C4-N3	-2.01	119.50	121.67

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	1519	MA6	O4'-C4'-C5'-O5'
43	1l	92	0TD	CA-CB-SB-CSB
43	1l	92	0TD	CG-CB-SB-CSB
55	1x	76	8AN	C3'-C4'-C5'-O5'
57	1y	46	G7M	C4'-C5'-O5'-P
32	2a	527	G7M	C3'-C4'-C5'-O5'
43	2l	92	0TD	CG-CB-SB-CSB
55	2x	76	8AN	O4'-C4'-C5'-O5'
55	2x	76	8AN	C3'-C4'-C5'-O5'
57	2y	54	5MU	C3'-C4'-C5'-O5'
57	2y	54	5MU	O4'-C4'-C5'-O5'
54	2w	32	PSU	C2'-C1'-C5-C4
54	1w	37	MIA	C12-C13-C14-C15
54	1w	37	MIA	C12-C13-C14-C16
32	1a	1519	MA6	C3'-C4'-C5'-O5'
32	2a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
57	2y	37	MIA	C3'-C4'-C5'-O5'
32	1a	1400	5MC	O4'-C4'-C5'-O5'
32	2a	1402	4OC	O4'-C4'-C5'-O5'
54	2w	46	G7M	C4'-C5'-O5'-P
32	1a	527	G7M	C3'-C4'-C5'-O5'
32	1a	1400	5MC	C3'-C4'-C5'-O5'
55	1x	76	8AN	O4'-C4'-C5'-O5'
32	2a	527	G7M	O4'-C4'-C5'-O5'
57	2y	37	MIA	O4'-C4'-C5'-O5'
54	2w	76	F3N	N-CA-CB-CG
54	1w	46	G7M	C4'-C5'-O5'-P
1	2A	2503	2MA	O4'-C4'-C5'-O5'
32	2a	1402	4OC	C3'-C4'-C5'-O5'
55	2x	76	8AN	C4'-C5'-O5'-P
32	2a	527	G7M	C4'-C5'-O5'-P
32	1a	527	G7M	O4'-C4'-C5'-O5'
54	2w	8	4SU	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
55	1x	76	8AN	C4'-C5'-O5'-P
32	2a	1519	MA6	C4'-C5'-O5'-P
54	2w	8	4SU	C3'-C4'-C5'-O5'
57	1y	8	4SU	C2'-C1'-N1-C6
54	1w	37	MIA	N6-C12-C13-C14
32	2a	1404	5MC	C3'-C4'-C5'-O5'
54	2w	46	G7M	C3'-C4'-C5'-O5'
57	1y	55	PSU	O4'-C1'-C5-C4
54	2w	39	PSU	O4'-C1'-C5-C4
1	1A	2503	2MA	C4'-C5'-O5'-P
43	2l	92	0TD	CA-CB-SB-CSB
54	2w	76	F3N	C-CA-CB-CG
57	1y	8	4SU	C2'-C1'-N1-C2
54	2w	32	PSU	O4'-C4'-C5'-O5'
1	1A	1915	5MU	O4'-C4'-C5'-O5'
54	2w	46	G7M	O4'-C4'-C5'-O5'
1	2A	2503	2MA	C3'-C4'-C5'-O5'
32	1a	1519	MA6	C4'-C5'-O5'-P
57	1y	55	PSU	O4'-C1'-C5-C6
57	2y	55	PSU	O4'-C1'-C5-C6
57	2y	8	4SU	C2'-C1'-N1-C2
43	2l	92	0TD	SB-CB-CG-OD1
1	1A	1920	OMC	C2'-C1'-N1-C2
32	2a	1402	4OC	C2'-C1'-N1-C2
1	1A	2503	2MA	O4'-C4'-C5'-O5'
57	1y	46	G7M	C3'-C4'-C5'-O5'
32	1a	527	G7M	C4'-C5'-O5'-P
57	2y	8	4SU	C2'-C1'-N1-C6

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 2778 ligands modelled in this entry, 2776 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	$\#\|Z\| > 2$
61	SF4	1d	302	35	0,12,12	-	-	-		
61	SF4	2d	303	35	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
61	SF4	1d	302	35	-	-	0/6/5/5
61	SF4	2d	303	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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	1A	2860/2915 (98%)	0.57	156 (5%)	25	24	14, 31, 78, 88	0
1	2A	2789/2915 (95%)	0.57	155 (5%)	24	23	28, 49, 76, 86	0
2	1B	120/121 (99%)	0.16	0	100	100	25, 43, 53, 73	0
2	2B	120/121 (99%)	0.28	2 (1%)	70	68	49, 61, 68, 79	0
3	1D	275/276 (99%)	0.61	2 (0%)	87	86	18, 34, 46, 62	0
3	2D	275/276 (99%)	0.81	2 (0%)	87	86	27, 44, 56, 71	0
4	1E	204/206 (99%)	0.54	0	100	100	14, 33, 53, 60	0
4	2E	204/206 (99%)	0.51	2 (0%)	82	80	28, 51, 60, 68	0
5	1F	202/210 (96%)	0.45	5 (2%)	57	55	15, 36, 58, 69	0
5	2F	202/210 (96%)	0.58	8 (3%)	38	37	28, 56, 66, 69	0
6	1G	181/182 (99%)	0.25	1 (0%)	89	88	33, 49, 60, 71	0
6	2G	181/182 (99%)	0.77	13 (7%)	15	14	52, 62, 70, 73	0
7	1H	174/180 (96%)	0.27	0	100	100	32, 46, 57, 69	0
7	2H	174/180 (96%)	2.00	74 (42%)	0	0	56, 67, 74, 78	0
8	1I	146/148 (98%)	0.46	2 (1%)	75	73	39, 60, 67, 72	0
8	2I	146/148 (98%)	0.92	19 (13%)	3	3	46, 64, 73, 77	0
9	1N	140/140 (100%)	0.42	0	100	100	20, 33, 50, 57	0
9	2N	140/140 (100%)	0.51	2 (1%)	75	73	41, 54, 65, 71	0
10	1O	122/122 (100%)	0.49	0	100	100	22, 35, 51, 57	0
10	2O	122/122 (100%)	0.44	1 (0%)	86	84	41, 51, 60, 65	0
11	1P	149/150 (99%)	0.34	2 (1%)	77	75	16, 40, 57, 63	0
11	2P	149/150 (99%)	0.88	15 (10%)	7	6	30, 55, 68, 73	0
12	1Q	141/141 (100%)	0.51	2 (1%)	75	73	22, 34, 47, 60	0
12	2Q	141/141 (100%)	0.66	4 (2%)	53	51	38, 54, 62, 64	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	1R	118/118 (100%)	0.41	0	100	100	18, 29, 40, 50	0
13	2R	118/118 (100%)	0.44	1 (0%)	86	84	35, 45, 54, 62	0
14	1S	110/112 (98%)	0.40	0	100	100	31, 42, 52, 58	0
14	2S	110/112 (98%)	0.76	12 (10%)	5	5	51, 59, 65, 68	0
15	1T	131/146 (89%)	0.27	0	100	100	25, 38, 59, 67	0
15	2T	131/146 (89%)	0.58	5 (3%)	40	39	41, 52, 61, 66	0
16	1U	116/118 (98%)	0.47	0	100	100	15, 25, 40, 47	0
16	2U	116/118 (98%)	0.64	4 (3%)	45	44	35, 49, 61, 67	0
17	1V	101/101 (100%)	0.29	0	100	100	17, 33, 48, 57	0
17	2V	101/101 (100%)	0.43	1 (0%)	82	80	35, 57, 63, 76	0
18	1W	112/113 (99%)	0.41	0	100	100	16, 26, 42, 65	0
18	2W	112/113 (99%)	0.48	0	100	100	34, 43, 53, 71	0
19	1X	95/96 (98%)	0.47	2 (2%)	63	61	23, 33, 49, 71	0
19	2X	95/96 (98%)	0.62	7 (7%)	14	13	39, 51, 64, 72	0
20	1Y	107/110 (97%)	0.28	1 (0%)	84	82	31, 42, 57, 66	0
20	2Y	107/110 (97%)	0.80	10 (9%)	8	8	51, 59, 68, 72	0
21	1Z	154/206 (74%)	0.64	15 (9%)	7	7	34, 53, 68, 73	0
21	2Z	160/206 (77%)	1.44	38 (23%)	0	0	51, 65, 73, 76	0
22	10	83/85 (97%)	0.50	1 (1%)	79	77	21, 32, 42, 54	0
22	20	83/85 (97%)	0.65	3 (3%)	42	42	33, 52, 60, 64	0
23	11	97/98 (98%)	0.37	1 (1%)	82	80	24, 41, 58, 61	0
23	21	97/98 (98%)	0.52	2 (2%)	63	61	33, 50, 62, 65	0
24	12	70/72 (97%)	0.36	0	100	100	30, 41, 50, 54	0
24	22	70/72 (97%)	0.69	5 (7%)	16	14	49, 59, 67, 76	0
25	13	59/60 (98%)	0.38	0	100	100	17, 30, 50, 56	0
25	23	59/60 (98%)	0.59	1 (1%)	70	68	46, 54, 62, 70	0
26	14	69/71 (97%)	0.66	9 (13%)	3	3	43, 61, 71, 79	0
26	24	69/71 (97%)	1.28	18 (26%)	0	0	61, 67, 75, 78	0
27	15	59/60 (98%)	0.52	1 (1%)	70	68	15, 25, 43, 52	0
27	25	59/60 (98%)	0.39	0	100	100	32, 43, 56, 66	0
28	16	53/54 (98%)	0.28	0	100	100	29, 37, 48, 52	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	26	53/54 (98%)	0.53	4 (7%) 14 13	39, 50, 58, 61	0
29	17	48/49 (97%)	0.58	1 (2%) 63 61	16, 22, 41, 52	0
29	27	48/49 (97%)	0.83	3 (6%) 20 18	28, 38, 58, 62	0
30	18	64/65 (98%)	0.42	0 100 100	23, 29, 36, 48	0
30	28	64/65 (98%)	0.53	1 (1%) 72 70	40, 47, 54, 57	0
31	19	37/37 (100%)	0.49	0 100 100	25, 33, 43, 48	0
31	29	37/37 (100%)	0.94	5 (13%) 3 2	48, 54, 59, 60	0
32	1a	1488/1521 (97%)	0.57	91 (6%) 21 20	32, 55, 75, 86	0
32	2a	1491/1521 (98%)	0.74	155 (10%) 6 6	43, 63, 77, 86	0
33	1b	231/256 (90%)	0.93	39 (16%) 1 1	50, 64, 70, 76	0
33	2b	231/256 (90%)	1.59	75 (32%) 0 0	59, 67, 73, 80	0
34	1c	206/239 (86%)	0.60	11 (5%) 26 25	49, 58, 65, 73	0
34	2c	206/239 (86%)	1.20	39 (18%) 1 1	57, 67, 73, 79	0
35	1d	208/209 (99%)	0.52	2 (0%) 82 80	45, 57, 64, 70	0
35	2d	208/209 (99%)	0.70	10 (4%) 30 29	49, 59, 66, 73	0
36	1e	148/162 (91%)	0.56	3 (2%) 65 63	44, 54, 62, 67	0
36	2e	148/162 (91%)	0.71	14 (9%) 8 7	53, 62, 66, 71	0
37	1f	100/101 (99%)	0.33	0 100 100	47, 56, 63, 65	0
37	2f	100/101 (99%)	0.37	0 100 100	48, 56, 63, 63	0
38	1g	155/156 (99%)	0.57	6 (3%) 39 38	51, 59, 69, 72	0
38	2g	155/156 (99%)	1.05	32 (20%) 1 0	56, 65, 70, 75	0
39	1h	137/138 (99%)	0.50	4 (2%) 51 50	48, 56, 62, 65	0
39	2h	137/138 (99%)	0.95	12 (8%) 10 9	53, 62, 68, 70	0
40	1i	127/128 (99%)	1.38	31 (24%) 0 0	48, 62, 68, 71	0
40	2i	127/128 (99%)	2.61	84 (66%) 0 0	57, 68, 72, 74	0
41	1j	97/105 (92%)	1.25	21 (21%) 0 0	47, 62, 69, 77	0
41	2j	96/105 (91%)	1.83	42 (43%) 0 0	57, 68, 72, 75	0
42	1k	114/129 (88%)	0.59	4 (3%) 44 43	35, 57, 63, 68	0
42	2k	114/129 (88%)	0.60	5 (4%) 34 33	48, 60, 66, 71	0
43	1l	121/132 (91%)	0.53	0 100 100	36, 45, 55, 60	0
43	2l	121/132 (91%)	0.47	0 100 100	46, 54, 62, 66	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
44	1m	123/126 (97%)	0.55	6 (4%)	29	28	46, 58, 66, 72	0
44	2m	122/126 (96%)	0.75	15 (12%)	4	3	57, 65, 69, 72	0
45	1n	60/61 (98%)	1.13	10 (16%)	1	1	49, 55, 61, 67	0
45	2n	60/61 (98%)	2.36	31 (51%)	0	0	60, 67, 71, 73	0
46	1o	88/89 (98%)	0.40	0	100	100	39, 53, 62, 67	0
46	2o	88/89 (98%)	0.49	3 (3%)	45	44	51, 59, 66, 69	0
47	1p	82/88 (93%)	0.84	10 (12%)	4	3	48, 58, 63, 69	0
47	2p	82/88 (93%)	0.87	7 (8%)	10	10	51, 58, 65, 68	0
48	1q	99/105 (94%)	0.76	9 (9%)	9	8	44, 57, 62, 69	0
48	2q	99/105 (94%)	1.08	17 (17%)	1	1	51, 59, 65, 67	0
49	1r	68/88 (77%)	0.38	4 (5%)	22	21	49, 56, 64, 66	0
49	2r	68/88 (77%)	0.31	2 (2%)	51	50	50, 58, 65, 67	0
50	1s	83/93 (89%)	0.40	3 (3%)	42	42	50, 58, 65, 68	0
50	2s	83/93 (89%)	1.08	13 (15%)	2	1	60, 66, 71, 74	0
51	1t	96/106 (90%)	1.42	25 (26%)	0	0	48, 58, 66, 71	0
51	2t	96/106 (90%)	1.48	27 (28%)	0	0	49, 59, 67, 71	0
52	1u	23/27 (85%)	1.50	5 (21%)	0	0	52, 56, 60, 62	0
52	2u	23/27 (85%)	2.31	13 (56%)	0	0	61, 65, 68, 71	0
53	1v	13/24 (54%)	1.04	3 (23%)	0	0	38, 44, 73, 76	0
53	2v	13/24 (54%)	1.60	5 (38%)	0	0	56, 61, 79, 89	0
54	1w	66/76 (86%)	0.81	7 (10%)	6	5	22, 69, 78, 84	0
54	2w	64/76 (84%)	1.13	9 (14%)	2	2	41, 74, 80, 86	0
55	1x	72/77 (93%)	0.35	0	100	100	21, 53, 68, 74	0
55	2x	72/77 (93%)	0.29	0	100	100	36, 62, 71, 78	0
56	1z	4/5 (80%)	0.67	0	100	100	22, 26, 31, 35	0
56	2z	3/5 (60%)	1.10	0	100	100	34, 34, 37, 40	0
57	1y	67/76 (88%)	3.53	58 (86%)	0	0	53, 80, 84, 85	0
57	2y	66/76 (86%)	3.70	57 (86%)	0	0	60, 80, 85, 86	0
All	All	20878/21758 (95%)	0.68	1637 (7%)	13	11	14, 54, 72, 89	0

All (1637) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
57	1y	5	G	9.4
57	1y	34	G	9.1
32	2a	1030(B)	C	9.0
1	2A	2160	G	9.0
1	2A	2127	G	9.0
1	1A	2131	G	8.4
54	1w	70	G	8.4
51	1t	95	ALA	8.4
21	2Z	149	SER	8.3
1	2A	2152	G	8.1
54	2w	71	G	7.9
21	2Z	155	LEU	7.9
1	1A	2159	G	7.7
57	2y	57	G	7.7
1	1A	2141	G	7.4
1	2A	2135	A	7.4
45	2n	38	GLY	7.3
40	2i	14	VAL	7.3
57	2y	36	A	7.3
44	1m	124	PRO	7.3
1	1A	2160	G	7.2
1	1A	2140	C	7.2
1	2A	2141	G	7.2
1	1A	2162	G	7.1
1	1A	2146	C	7.1
32	1a	1001(A)	G	7.0
1	2A	2115	G	6.9
21	2Z	141	VAL	6.7
1	2A	2128	C	6.7
1	2A	2116	G	6.6
1	2A	2126	A	6.6
1	2A	2123	G	6.6
57	1y	35	A	6.6
1	2A	2161	C	6.5
33	2b	207	ALA	6.5
40	2i	45	ALA	6.5
1	1A	2181	G	6.5
1	2A	883	G	6.4
32	2a	1030(A)	G	6.4
32	2a	1031	G	6.4
1	2A	2140	C	6.4
7	2H	35	VAL	6.4
57	1y	19	G	6.4

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Mol	Chain	Res	Type	RSRZ
1	1A	2129	C	6.3
1	2A	884	C	6.3
20	2Y	55	TYR	6.3
1	2A	2169	A	6.3
57	1y	36	A	6.3
38	1g	156	TRP	6.2
26	24	51	ASP	6.2
33	2b	37	ASN	6.2
1	1A	2161	C	6.1
54	2w	70	G	6.1
57	2y	65	G	6.1
57	2y	56	C	6.1
1	1A	2142	C	6.1
1	2A	885	C	6.1
32	2a	1033	G	6.1
57	1y	13	C	6.1
38	2g	40	ALA	6.1
57	2y	29	G	6.0
1	1A	897	C	6.0
1	1A	2130	U	6.0
1	2A	2170	A	6.0
26	24	63	TYR	6.0
1	2A	2125	G	5.9
57	2y	62	C	5.9
57	2y	64	A	5.9
1	1A	2182	G	5.9
1	2A	2159	G	5.9
57	2y	1	G	5.9
26	24	66	SER	5.9
1	2A	2136	C	5.9
1	2A	888	C	5.9
1	2A	2139	C	5.9
1	1A	896	A	5.9
7	2H	92	ILE	5.9
45	2n	25	VAL	5.8
45	2n	43	CYS	5.8
32	2a	1001(A)	G	5.7
32	2a	1447	A	5.7
57	2y	19	G	5.7
1	1A	2147	G	5.7
1	2A	229	A	5.7
40	2i	65	VAL	5.6

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Mol	Chain	Res	Type	RSRZ
32	2a	1452	C	5.6
57	2y	75	C	5.6
1	2A	2112	G	5.6
1	2A	896	A	5.6
57	2y	66	U	5.6
57	1y	22	G	5.6
1	1A	2145	C	5.6
40	2i	76	ALA	5.5
40	2i	88	TYR	5.5
54	1w	71	G	5.5
21	2Z	153	SER	5.5
1	1A	2164	C	5.5
1	2A	2162	G	5.5
34	2c	87	LEU	5.5
1	2A	2134	A	5.4
1	2A	1041	C	5.4
32	2a	1026	G	5.4
7	2H	6	ARG	5.4
44	1m	123	ALA	5.4
1	2A	2124	G	5.4
57	1y	57	G	5.4
1	1A	893	C	5.4
1	2A	2117	A	5.3
57	2y	44	G	5.3
1	1A	2109	U	5.3
39	2h	58	TYR	5.3
1	1A	1059	G	5.2
1	2A	2120	G	5.2
32	2a	1030(C)	G	5.2
1	1A	2144	U	5.2
7	2H	113	VAL	5.2
57	2y	38	A	5.2
40	2i	27	THR	5.2
33	2b	122	PHE	5.2
32	2a	1286	A	5.2
1	1A	2128	C	5.2
57	1y	24	G	5.2
57	2y	52	G	5.2
35	2d	6	GLY	5.2
32	1a	1028	C	5.1
45	2n	42	ILE	5.1
1	1A	2148	G	5.1

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Mol	Chain	Res	Type	RSRZ
34	2c	160	ALA	5.1
1	1A	2133	G	5.1
32	1a	1001	A	5.1
7	2H	98	LEU	5.1
41	2j	88	LEU	5.1
1	2A	2138	C	5.1
32	2a	1034	G	5.1
1	1A	2132	U	5.1
1	2A	2167	U	5.1
7	2H	105	LEU	5.1
1	2A	2121	G	5.0
32	1a	1032	G	5.0
44	2m	124	PRO	5.0
45	2n	61	TRP	5.0
1	2A	2147	G	5.0
1	1A	1509	C	5.0
1	2A	2149	G	5.0
1	2A	2154	G	5.0
57	1y	71	G	5.0
32	1a	1257	U	5.0
1	2A	2142	C	5.0
1	2A	2171	A	5.0
32	2a	1256	A	5.0
57	1y	38	A	4.9
41	1j	18	ALA	4.9
57	1y	18	G	4.9
32	2a	1030	C	4.9
32	2a	1446	U	4.9
1	1A	2120	G	4.9
32	2a	1036	G	4.9
45	2n	26	ARG	4.9
32	1a	1040	U	4.9
1	2A	2133	G	4.9
1	2A	2174	C	4.9
40	2i	28	VAL	4.9
57	2y	14	A	4.9
51	1t	47	GLY	4.8
57	2y	45	U	4.8
1	1A	2794	C	4.8
1	2A	2168	G	4.8
21	2Z	51	ALA	4.8
38	2g	156	TRP	4.8

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Mol	Chain	Res	Type	RSRZ
1	1A	2166	G	4.8
1	1A	2127	G	4.8
33	2b	81	VAL	4.8
7	2H	36	PRO	4.8
33	2b	44	LEU	4.8
21	1Z	164	ALA	4.8
1	2A	2129	C	4.8
5	1F	16	GLY	4.7
32	2a	80	G	4.7
21	2Z	170	THR	4.7
38	1g	81	GLY	4.7
1	2A	895	U	4.7
57	1y	53	G	4.7
33	2b	230	VAL	4.7
53	2v	12	A	4.7
57	2y	21	A	4.7
7	2H	72	ILE	4.7
26	14	54	GLY	4.7
32	1a	1031	G	4.7
1	1A	1064	C	4.7
33	2b	165	VAL	4.7
52	2u	24	ARG	4.7
1	1A	1063	G	4.7
32	2a	216	G	4.7
57	2y	43	C	4.7
33	2b	34	ALA	4.7
1	2A	1114	G	4.7
1	2A	2113	U	4.6
1	2A	2802	G	4.6
57	2y	63	G	4.6
11	2P	101	VAL	4.6
21	2Z	58	VAL	4.6
33	2b	112	VAL	4.6
1	2A	1026	U	4.6
34	2c	92	ALA	4.6
34	2c	94	LEU	4.6
34	1c	81	GLY	4.6
1	2A	2166	G	4.6
40	2i	90	PRO	4.6
52	2u	14	TRP	4.6
1	1A	2165	G	4.6
21	2Z	139	VAL	4.6

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Mol	Chain	Res	Type	RSRZ
32	1a	1033	G	4.6
32	1a	1041	A	4.6
32	1a	1447	A	4.6
57	1y	67	C	4.5
6	2G	29	TRP	4.5
33	1b	227	GLY	4.5
40	2i	30	GLY	4.5
40	2i	109	VAL	4.5
34	2c	157	ILE	4.5
21	2Z	144	LEU	4.5
32	1a	216	G	4.5
57	1y	70	G	4.5
32	1a	204	U	4.5
40	2i	80	GLY	4.5
26	24	50	VAL	4.5
57	2y	33	U	4.5
32	2a	1041	A	4.5
32	1a	1446	U	4.4
1	1A	2114	A	4.4
51	2t	9	ASN	4.4
57	1y	1	G	4.4
1	2A	2143	C	4.4
1	2A	2146	C	4.4
32	1a	1030(C)	G	4.4
32	2a	1249	C	4.4
33	2b	127	ILE	4.4
57	2y	67	C	4.4
32	2a	1150	U	4.4
7	2H	71	LEU	4.4
26	24	29	PRO	4.4
57	2y	42	C	4.4
33	1b	123	ALA	4.4
1	1A	2112	G	4.4
1	2A	652(U)	G	4.4
1	1A	1095	A	4.4
1	1A	271(K)	U	4.4
40	2i	36	TYR	4.4
1	1A	1076	C	4.4
9	2N	9	VAL	4.4
24	22	70	GLN	4.4
8	2I	59	ALA	4.3
32	2a	1287	A	4.3

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Mol	Chain	Res	Type	RSRZ
1	2A	898	C	4.3
5	2F	15	SER	4.3
27	15	60	VAL	4.3
52	2u	17	THR	4.3
32	2a	1024	G	4.3
32	1a	841	U	4.3
32	2a	1250	A	4.3
1	2A	2175	C	4.3
50	2s	50	ALA	4.3
40	2i	62	TYR	4.3
32	1a	1029	C	4.3
1	2A	2151	G	4.3
32	1a	1003	G	4.3
57	2y	5	G	4.3
1	1A	2108	C	4.3
7	2H	44	VAL	4.3
51	1t	45	GLN	4.3
1	1A	899	A	4.3
48	2q	80	GLY	4.3
21	2Z	96	VAL	4.3
54	1w	44	G	4.3
1	1A	2117	A	4.2
1	2A	2145	C	4.2
7	2H	121	ILE	4.2
1	1A	887	A	4.2
1	1A	892	G	4.2
1	1A	889	C	4.2
1	2A	2114	A	4.2
45	2n	55	GLY	4.2
40	2i	105	ASP	4.2
21	2Z	152	ALA	4.2
1	1A	2185	C	4.2
1	2A	892	G	4.2
1	2A	1040	C	4.2
57	2y	28	G	4.2
57	2y	34	G	4.2
57	2y	74	C	4.2
45	1n	13	THR	4.2
1	2A	2144	U	4.2
57	1y	12	U	4.2
1	2A	2163	C	4.2
33	1b	134	GLU	4.2

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Mol	Chain	Res	Type	RSRZ
57	2y	58	A	4.2
1	2A	2110	G	4.2
8	2I	74	ASN	4.2
1	1A	1175	U	4.2
32	2a	1257	U	4.2
41	2j	19	SER	4.2
21	2Z	106	GLY	4.1
21	2Z	147	GLY	4.1
1	1A	229	A	4.1
1	1A	2174	C	4.1
32	2a	1029	C	4.1
40	2i	31	GLN	4.1
57	2y	69	G	4.1
1	2A	2177	C	4.1
32	2a	91	C	4.1
1	1A	278	A	4.1
57	1y	21	A	4.1
45	2n	24	CYS	4.1
32	2a	204	U	4.1
40	2i	108	VAL	4.1
1	1A	2792	G	4.1
1	2A	11	G	4.1
51	1t	100	ILE	4.1
1	1A	1072	C	4.1
8	2I	75	LEU	4.1
40	1i	49	PRO	4.1
40	2i	67	GLY	4.1
1	1A	2110	G	4.1
32	2a	1032	G	4.1
32	2a	1154	G	4.1
1	2A	894	C	4.1
1	2A	2164	C	4.1
21	2Z	159	PRO	4.1
33	2b	236	TYR	4.1
34	2c	100	ALA	4.1
38	2g	6	ARG	4.1
40	1i	81	ILE	4.0
33	2b	232	PRO	4.0
33	2b	233	SER	4.0
57	1y	4	C	4.0
1	1A	2158	A	4.0
11	2P	103	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
57	1y	23	A	4.0
1	1A	2106	G	4.0
1	2A	2153	G	4.0
32	1a	1030(B)	C	4.0
32	2a	1006	C	4.0
51	2t	99	LEU	4.0
57	1y	20	U	4.0
1	1A	2156	G	4.0
32	2a	1023	G	4.0
57	1y	30	G	4.0
40	1i	98	PRO	4.0
32	2a	1007	C	4.0
1	2A	2158	A	4.0
32	2a	1248	A	4.0
41	2j	47	PHE	4.0
41	2j	67	THR	4.0
24	22	58	ALA	4.0
1	1A	2168	G	4.0
1	2A	1039	G	4.0
1	2A	2157	G	4.0
32	2a	1035	A	4.0
33	2b	220	ASP	4.0
45	2n	13	THR	4.0
40	2i	9	ARG	3.9
1	2A	2148	G	3.9
53	2v	24	A	3.9
40	2i	15	ALA	3.9
45	2n	37	PHE	3.9
1	2A	887	A	3.9
1	2A	2106	G	3.9
40	1i	80	GLY	3.9
40	2i	8	GLY	3.9
7	2H	16	SER	3.9
14	2S	20	ARG	3.9
50	2s	41	VAL	3.9
1	2A	2122	U	3.9
57	1y	61	C	3.9
7	2H	75	ALA	3.9
34	2c	155	GLY	3.9
38	2g	154	TYR	3.9
7	2H	70	THR	3.9
40	2i	103	THR	3.9

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Mol	Chain	Res	Type	RSRZ
1	1A	2188	C	3.9
20	2Y	65	ALA	3.9
57	1y	45	U	3.9
41	2j	11	PHE	3.9
7	2H	106	THR	3.9
33	2b	48	MET	3.9
1	1A	888	C	3.9
1	1A	2135	A	3.9
40	1i	19	LEU	3.9
51	2t	41	ILE	3.9
36	1e	69	VAL	3.9
40	2i	35	GLU	3.9
50	2s	30	LEU	3.9
33	2b	113	HIS	3.8
32	1a	1023	G	3.8
1	1A	2139	C	3.8
51	2t	47	GLY	3.8
41	2j	74	ILE	3.8
5	2F	115	ALA	3.8
41	2j	20	ALA	3.8
21	1Z	166	SER	3.8
32	1a	202	U	3.8
32	1a	1030(A)	G	3.8
32	2a	1002	G	3.8
32	2a	1260	C	3.8
32	1a	1030(D)	A	3.8
57	1y	58	A	3.8
36	2e	32	VAL	3.8
1	1A	2155	G	3.8
1	2A	2165	G	3.8
32	1a	1026	G	3.8
52	2u	9	ARG	3.8
33	2b	17	PHE	3.8
7	2H	20	ALA	3.8
40	2i	94	ALA	3.8
40	2i	72	GLY	3.8
32	1a	1024	G	3.8
40	1i	61	ALA	3.8
40	2i	63	ILE	3.8
41	2j	98	ILE	3.8
57	2y	68	C	3.8
1	1A	1065	U	3.8

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Mol	Chain	Res	Type	RSRZ
1	1A	890	A	3.8
57	2y	23	A	3.8
19	2X	1	MET	3.8
1	1A	2126	A	3.8
1	2A	652(B)	A	3.8
1	2A	2119	A	3.8
33	2b	210	SER	3.8
52	2u	8	THR	3.8
51	2t	57	ARG	3.7
47	2p	58	TYR	3.7
1	2A	2137	C	3.7
57	1y	49	C	3.7
1	1A	2154	G	3.7
57	2y	30	G	3.7
45	2n	40	CYS	3.7
51	2t	44	ALA	3.7
34	2c	39	ILE	3.7
1	2A	2895	U	3.7
19	2X	92	LEU	3.7
1	1A	2123	G	3.7
1	1A	2152	G	3.7
32	2a	79	G	3.7
33	2b	216	SER	3.7
1	1A	2175	C	3.7
32	1a	217	C	3.7
26	14	66	SER	3.7
7	2H	24	VAL	3.7
21	1Z	165	VAL	3.7
40	1i	100	GLY	3.7
26	24	49	PHE	3.7
57	1y	64	A	3.7
57	2y	35	A	3.7
52	2u	23	PRO	3.7
7	2H	79	VAL	3.7
32	1a	1037	C	3.7
1	2A	2182	G	3.7
57	1y	69	G	3.7
57	2y	18	G	3.7
21	2Z	62	PRO	3.7
41	2j	72	VAL	3.7
33	2b	14	GLY	3.6
7	2H	128	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
32	2a	1157	A	3.6
1	2A	2156	G	3.6
32	1a	1036	G	3.6
40	2i	86	VAL	3.6
32	2a	1028	C	3.6
32	2a	1116	C	3.6
1	2A	2172	U	3.6
38	1g	79	ARG	3.6
33	1b	233	SER	3.6
45	2n	34	TYR	3.6
32	1a	1286	A	3.6
32	2a	1283	G	3.6
41	2j	36	GLY	3.6
32	2a	1532	U	3.6
7	2H	169	VAL	3.6
32	1a	1000	U	3.6
40	2i	49	PRO	3.6
33	2b	16	HIS	3.6
40	1i	109	VAL	3.6
1	2A	2173	A	3.6
1	2A	2801(A)	A	3.6
14	2S	22	GLY	3.6
33	1b	228	GLY	3.6
41	2j	96	ILE	3.6
26	14	18	CYS	3.6
32	2a	1040	U	3.6
1	2A	277	C	3.6
57	1y	3	C	3.6
57	1y	52	G	3.6
57	2y	24	G	3.6
40	2i	87	GLN	3.6
1	1A	2113	U	3.6
40	2i	66	ARG	3.6
1	2A	897	C	3.6
32	2a	1039	C	3.6
45	2n	44	LEU	3.6
1	1A	1074	G	3.6
1	1A	2184	G	3.6
32	2a	1003	G	3.6
32	2a	1156	G	3.6
48	1q	7	THR	3.6
11	2P	110	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
39	2h	65	TYR	3.6
51	1t	67	ALA	3.6
21	1Z	141	VAL	3.6
41	1j	38	ILE	3.5
47	1p	66	PRO	3.5
7	2H	91	GLY	3.5
21	2Z	148	ASP	3.5
41	2j	15	THR	3.5
57	1y	56	C	3.5
6	2G	50	ALA	3.5
40	2i	82	ALA	3.5
39	1h	53	VAL	3.5
41	2j	86	MET	3.5
41	1j	47	PHE	3.5
45	2n	14	PRO	3.5
32	2a	1358	U	3.5
36	2e	62	ALA	3.5
57	1y	74	C	3.5
1	1A	879	G	3.5
1	2A	2104	G	3.5
57	2y	50	U	3.5
31	29	29	ASN	3.5
1	1A	884	C	3.5
8	1I	136	VAL	3.5
32	2a	999	C	3.5
40	2i	4	TYR	3.5
32	1a	1138	G	3.5
50	2s	68	GLY	3.5
57	1y	15	G	3.5
33	2b	51	LEU	3.5
45	2n	36	PHE	3.5
1	1A	2115	G	3.5
40	2i	122	ALA	3.5
7	2H	111	HIS	3.5
41	2j	13	HIS	3.5
38	2g	80	VAL	3.5
53	1v	12	A	3.5
51	1t	38	LYS	3.5
1	1A	895	U	3.5
38	2g	108	ALA	3.5
1	1A	1099	G	3.5
1	1A	2805	G	3.5

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Mol	Chain	Res	Type	RSRZ
1	2A	2155	G	3.5
32	2a	1245	A	3.4
40	2i	33	PHE	3.4
1	2A	652(T)	C	3.4
40	1i	117	HIS	3.4
50	1s	72	GLY	3.4
28	26	52	VAL	3.4
1	1A	2151	G	3.4
1	2A	614(B)	G	3.4
57	2y	53	G	3.4
57	1y	62	C	3.4
44	2m	49	THR	3.4
33	2b	235	SER	3.4
6	2G	149	VAL	3.4
40	1i	14	VAL	3.4
40	2i	53	VAL	3.4
1	2A	2793	G	3.4
57	1y	44	G	3.4
40	2i	102	LEU	3.4
33	2b	116	GLU	3.4
45	1n	2	ALA	3.4
40	2i	93	ARG	3.4
45	2n	12	ARG	3.4
7	2H	43	VAL	3.4
44	1m	25	ILE	3.4
1	2A	2109	U	3.4
1	2A	274	G	3.4
1	2A	890	A	3.4
32	1a	93	G	3.4
32	2a	1022	G	3.4
33	1b	18	GLY	3.4
36	2e	138	ALA	3.4
40	2i	57	GLY	3.4
38	2g	9	VAL	3.4
34	2c	182	ILE	3.4
7	2H	74	ASN	3.4
32	1a	1025	U	3.4
34	2c	145	GLY	3.4
40	2i	19	LEU	3.4
40	1i	90	PRO	3.4
32	1a	145	G	3.4
32	2a	1284	C	3.4

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Mol	Chain	Res	Type	RSRZ
39	2h	71	GLY	3.4
48	1q	27	PHE	3.4
7	2H	21	PRO	3.4
21	1Z	169	GLU	3.4
21	1Z	1	MET	3.4
47	2p	1	MET	3.4
1	1A	2170	A	3.4
7	2H	25	LYS	3.4
36	2e	34	VAL	3.4
57	1y	42	C	3.4
7	2H	51	ARG	3.4
57	1y	75	C	3.3
11	2P	91	PHE	3.3
41	1j	96	ILE	3.3
36	2e	104	ALA	3.3
38	2g	24	THR	3.3
41	2j	44	VAL	3.3
1	2A	1117	G	3.3
1	2A	2319	G	3.3
42	1k	15	ALA	3.3
45	2n	22	THR	3.3
52	1u	17	THR	3.3
8	2I	57	ARG	3.3
57	2y	70	G	3.3
26	14	63	TYR	3.3
1	2A	645	C	3.3
33	2b	47	THR	3.3
52	2u	13	ILE	3.3
32	2a	1155	G	3.3
33	2b	92	TYR	3.3
57	2y	15	G	3.3
40	2i	91	ASP	3.3
6	2G	3	LEU	3.3
1	1A	1054	A	3.3
1	2A	2130	U	3.3
14	2S	66	ALA	3.3
32	1a	162	A	3.3
33	2b	19	HIS	3.3
45	2n	35	ARG	3.3
45	2n	39	LEU	3.3
32	2a	202	U	3.3
1	1A	2790	A	3.3

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Mol	Chain	Res	Type	RSRZ
1	2A	1116	C	3.3
32	1a	999	C	3.3
32	2a	1030(D)	A	3.3
32	2a	1531	A	3.3
40	2i	54	ASP	3.3
39	2h	19	VAL	3.3
1	1A	2149	G	3.2
7	2H	112	PRO	3.2
22	20	62	LEU	3.2
33	1b	118	LEU	3.2
40	2i	56	LEU	3.2
7	2H	82	GLY	3.2
40	2i	61	ALA	3.2
32	1a	1039	C	3.2
50	2s	45	VAL	3.2
39	2h	36	LEU	3.2
7	2H	123	PHE	3.2
34	2c	61	ALA	3.2
32	1a	79	G	3.2
32	2a	1027	C	3.2
54	2w	72	C	3.2
57	2y	73	A	3.2
33	2b	102	LEU	3.2
14	2S	5	THR	3.2
33	2b	214	ILE	3.2
32	1a	1007	C	3.2
32	2a	1130	A	3.2
52	1u	2	GLY	3.2
8	2I	83	ALA	3.2
1	1A	2180	U	3.2
14	2S	31	SER	3.2
40	2i	51	ARG	3.2
1	1A	2186	G	3.2
1	2A	2181	G	3.2
32	1a	198	G	3.2
32	2a	1456	G	3.2
29	17	46	VAL	3.2
32	1a	201	C	3.2
32	2a	217	C	3.2
40	1i	31	GLN	3.2
1	1A	1060	U	3.2
40	2i	115	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	1A	2125	G	3.2
1	2A	652(V)	C	3.2
1	2A	2179	C	3.2
40	2i	5	TYR	3.2
45	2n	10	ALA	3.2
1	1A	2102	U	3.2
34	1c	41	GLY	3.2
23	21	68	PRO	3.2
34	2c	48	TYR	3.1
50	2s	63	THR	3.1
51	2t	95	ALA	3.1
1	1A	2116	G	3.1
32	2a	998	G	3.1
1	1A	1057	A	3.1
7	2H	126	PRO	3.1
21	2Z	156	LYS	3.1
33	1b	125	PRO	3.1
11	2P	92	GLU	3.1
34	2c	198	VAL	3.1
33	1b	236	TYR	3.1
1	2A	1113	U	3.1
20	2Y	61	ILE	3.1
34	2c	93	LYS	3.1
44	2m	4	ILE	3.1
45	2n	51	GLY	3.1
1	1A	1056	G	3.1
53	1v	14	A	3.1
33	1b	21	ARG	3.1
8	2I	63	ALA	3.1
34	2c	60	ALA	3.1
1	1A	2118	U	3.1
20	2Y	1	MET	3.1
41	2j	68	HIS	3.1
32	1a	840	C	3.1
32	2a	1115	C	3.1
1	2A	1042	G	3.1
1	2A	1115	G	3.1
8	2I	81	VAL	3.1
39	2h	124	ALA	3.1
7	2H	8	PRO	3.1
1	1A	894	C	3.1
33	2b	132	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	2A	275	G	3.1
32	2a	1258	G	3.1
7	2H	32	GLU	3.1
35	2d	115	ARG	3.1
41	2j	40	LEU	3.1
33	2b	228	GLY	3.1
33	2b	105	PHE	3.1
33	2b	201	ILE	3.1
41	1j	4	ILE	3.1
1	1A	2803	C	3.1
57	1y	2	C	3.1
40	2i	121	ARG	3.1
32	2a	1251	A	3.1
40	2i	44	VAL	3.1
1	1A	2157	G	3.1
32	1a	78	G	3.1
32	2a	1009	G	3.1
31	29	30	PRO	3.1
57	1y	47	U	3.1
40	2i	20	ARG	3.1
1	1A	2143	C	3.1
52	1u	16	GLY	3.1
33	2b	120	ALA	3.1
38	2g	22	LEU	3.1
40	2i	7	THR	3.1
7	2H	45	VAL	3.1
50	1s	58	VAL	3.1
53	1v	13	A	3.0
57	1y	6	G	3.0
57	2y	51	U	3.0
7	2H	48	GLY	3.0
11	2P	138	LEU	3.0
41	1j	62	HIS	3.0
48	2q	7	THR	3.0
1	1A	1098	A	3.0
1	1A	1082	U	3.0
50	2s	80	TYR	3.0
1	2A	2131	G	3.0
32	1a	138	G	3.0
32	1a	1034	G	3.0
32	2a	1202	G	3.0
32	2a	1443	G	3.0

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Mol	Chain	Res	Type	RSRZ
51	2t	26	ASN	3.0
7	2H	102	ALA	3.0
1	2A	876	C	3.0
1	2A	889	C	3.0
48	1q	36	ILE	3.0
52	2u	16	GLY	3.0
23	21	2	SER	3.0
40	2i	123	PRO	3.0
7	2H	167	GLU	3.0
32	2a	203	U	3.0
34	2c	159	GLY	3.0
44	1m	26	GLY	3.0
33	1b	137	ARG	3.0
33	1b	207	ALA	3.0
33	1b	221	LEU	3.0
38	2g	46	ALA	3.0
1	2A	2107	C	3.0
32	1a	163	C	3.0
32	1a	1137	C	3.0
26	24	59	PHE	3.0
32	1a	96	U	3.0
33	2b	223	ILE	3.0
41	2j	89	ASP	3.0
21	2Z	2	GLU	3.0
40	2i	114	TYR	3.0
33	1b	187	LEU	3.0
36	2e	146	ALA	3.0
40	1i	94	ALA	3.0
7	2H	12	PRO	3.0
39	2h	67	PRO	3.0
33	1b	229	VAL	3.0
45	2n	18	VAL	3.0
48	2q	92	ARG	3.0
1	1A	1092	C	3.0
11	2P	94	GLU	3.0
8	2I	46	ALA	3.0
38	2g	25	ALA	3.0
54	2w	31	A	3.0
32	2a	1278	U	2.9
51	2t	100	ILE	2.9
57	1y	59	U	2.9
1	1A	2178	C	2.9

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Mol	Chain	Res	Type	RSRZ
1	2A	1509	C	2.9
57	2y	6	G	2.9
34	2c	23	TYR	2.9
34	2c	33	LEU	2.9
35	2d	168	ARG	2.9
40	1i	10	ARG	2.9
41	2j	69	ASN	2.9
33	2b	129	GLU	2.9
36	2e	33	VAL	2.9
48	2q	73	VAL	2.9
50	2s	13	ASP	2.9
8	2I	143	SER	2.9
11	2P	102	ARG	2.9
41	2j	29	ARG	2.9
32	2a	1008	C	2.9
57	2y	25	C	2.9
33	1b	138	LEU	2.9
35	2d	162	LEU	2.9
48	2q	22	LEU	2.9
1	1A	1084	A	2.9
1	1A	2119	A	2.9
7	2H	99	VAL	2.9
7	2H	47	GLU	2.9
7	2H	148	ILE	2.9
33	2b	211	ILE	2.9
54	1w	20	U	2.9
33	1b	120	ALA	2.9
40	1i	84	ALA	2.9
41	1j	26	ALA	2.9
1	2A	2896	C	2.9
41	2j	8	LEU	2.9
47	1p	60	LEU	2.9
57	2y	2	C	2.9
34	1c	193	TYR	2.9
52	2u	21	TYR	2.9
1	1A	882	G	2.9
32	1a	1021	G	2.9
32	2a	1224	G	2.9
1	1A	1096	A	2.9
33	2b	91	PRO	2.9
6	2G	62	LEU	2.9
14	2S	56	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
51	1t	91	LEU	2.9
1	1A	2103	C	2.9
32	2a	1149	C	2.9
33	1b	133	LYS	2.9
26	24	45	GLY	2.9
32	2a	1122	U	2.9
45	1n	7	ILE	2.9
57	2y	26	A	2.9
7	2H	33	LEU	2.9
7	2H	165	ALA	2.9
26	14	55	ARG	2.9
50	1s	5	LEU	2.9
32	2a	150	C	2.9
7	2H	125	VAL	2.9
20	2Y	5	MET	2.9
40	1i	57	GLY	2.9
1	2A	272(A)	U	2.9
1	2A	877	U	2.9
1	2A	2132	U	2.9
32	2a	839	U	2.9
32	2a	1142	G	2.9
1	1A	2169	A	2.9
51	2t	98	PRO	2.9
40	2i	70	LYS	2.9
40	2i	73	GLN	2.9
7	2H	65	HIS	2.9
40	1i	4	TYR	2.9
33	2b	15	VAL	2.8
1	1A	1066	U	2.8
1	1A	2167	U	2.8
1	1A	2187	G	2.8
1	2A	2100	G	2.8
32	1a	1002	G	2.8
44	1m	2	ALA	2.8
45	1n	12	ARG	2.8
47	1p	78	GLY	2.8
51	1t	70	SER	2.8
1	2A	2183	C	2.8
1	2A	2803	C	2.8
32	2a	174	C	2.8
54	1w	72	C	2.8
57	1y	11	C	2.8

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Mol	Chain	Res	Type	RSRZ
1	2A	9	U	2.8
34	2c	124	ILE	2.8
57	2y	59	U	2.8
38	2g	83	ALA	2.8
41	2j	100	THR	2.8
51	2t	73	HIS	2.8
7	2H	7	LEU	2.8
7	2H	31	GLY	2.8
7	2H	11	VAL	2.8
7	2H	19	VAL	2.8
36	2e	90	VAL	2.8
21	1Z	133	ILE	2.8
32	1a	1006	C	2.8
33	2b	86	GLU	2.8
57	2y	47	U	2.8
40	2i	52	ALA	2.8
33	1b	37	ASN	2.8
1	1A	2793	G	2.8
32	1a	144	G	2.8
32	2a	145	G	2.8
32	2a	378	G	2.8
34	2c	193	TYR	2.8
32	2a	1259	C	2.8
34	2c	74	GLY	2.8
35	2d	167	GLY	2.8
7	2H	2	SER	2.8
21	2Z	126	VAL	2.8
32	1a	171	A	2.8
32	2a	1180	A	2.8
32	2a	1349	A	2.8
1	2A	2180	U	2.8
32	1a	1136	U	2.8
44	2m	9	ILE	2.8
57	1y	60	U	2.8
38	2g	5	ARG	2.8
1	1A	2171	A	2.8
21	1Z	154	ASP	2.8
21	2Z	140	ASP	2.8
45	2n	56	VAL	2.8
14	2S	92	TYR	2.8
24	22	24	LEU	2.8
32	2a	1061	G	2.8

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Mol	Chain	Res	Type	RSRZ
57	1y	48	C	2.8
34	1c	86	VAL	2.7
36	2e	20	GLN	2.7
1	2A	2150	U	2.7
33	2b	75	LYS	2.7
33	2b	203	GLY	2.7
38	2g	81	GLY	2.7
5	1F	13	SER	2.7
32	2a	1323	G	2.7
32	2a	1370	G	2.7
1	1A	898	C	2.7
1	2A	886	C	2.7
15	2T	124	ASP	2.7
33	2b	133	LYS	2.7
42	1k	14	VAL	2.7
7	2H	94	TYR	2.7
51	2t	94	ALA	2.7
32	2a	1005	A	2.7
32	2a	1275	A	2.7
57	1y	14	A	2.7
33	2b	231	GLU	2.7
40	2i	2	GLU	2.7
48	1q	78	GLU	2.7
41	2j	22	LYS	2.7
1	1A	880	G	2.7
1	2A	272(J)	C	2.7
1	2A	2108	C	2.7
12	1Q	55	VAL	2.7
52	1u	15	ARG	2.7
13	2R	62	ALA	2.7
15	2T	110	ILE	2.7
32	2a	90	U	2.7
36	2e	21	ALA	2.7
38	2g	147	ALA	2.7
42	1k	64	ALA	2.7
51	1t	44	ALA	2.7
34	2c	184	TYR	2.7
48	2q	39	SER	2.7
6	2G	138	GLN	2.7
40	2i	29	ASN	2.7
40	2i	107	ARG	2.7
52	2u	22	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
57	2y	61	C	2.7
16	2U	63	VAL	2.7
32	2a	1292	U	2.7
40	2i	46	ALA	2.7
21	2Z	57	ILE	2.7
33	1b	135	GLN	2.7
41	1j	33	GLN	2.7
51	1t	92	LEU	2.7
1	2A	2103	C	2.7
41	2j	34	VAL	2.7
1	2A	2189	U	2.7
23	1l	2	SER	2.7
32	1a	1212	U	2.7
34	1c	189	ALA	2.7
50	2s	79	THR	2.7
57	2y	12	U	2.7
1	2A	2191	G	2.7
32	2a	198	G	2.7
32	2a	1442	G	2.7
32	2a	1442(A)	G	2.7
33	1b	222	ILE	2.7
33	2b	152	PHE	2.7
40	2i	99	LEU	2.7
57	2y	71	G	2.7
8	2I	113	ARG	2.7
32	1a	1157	A	2.7
32	2a	383	A	2.7
25	23	56	VAL	2.7
42	2k	14	VAL	2.7
1	1A	2111	C	2.7
1	1A	2136	C	2.7
9	2N	10	GLU	2.7
32	2a	218	C	2.7
45	2n	46	GLU	2.7
35	2d	70	ILE	2.7
51	1t	80	ARG	2.7
32	1a	998	G	2.7
32	2a	1021	G	2.7
32	2a	1353	G	2.7
34	2c	185	GLY	2.7
54	2w	15	G	2.7
57	1y	63	G	2.7

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Mol	Chain	Res	Type	RSRZ
32	2a	1001	A	2.6
3	1D	2	ALA	2.6
14	2S	3	ARG	2.6
33	2b	85	ALA	2.6
51	2t	59	ALA	2.6
1	2A	893	C	2.6
32	2a	189(D)	C	2.6
35	2d	11	LEU	2.6
7	2H	83	TYR	2.6
1	1A	2153	G	2.6
32	1a	61	G	2.6
32	2a	1274	G	2.6
32	2a	1356	G	2.6
33	2b	30	ARG	2.6
17	2V	72	VAL	2.6
41	2j	24	VAL	2.6
47	2p	2	VAL	2.6
34	1c	15	THR	2.6
47	1p	7	ALA	2.6
19	2X	94	GLY	2.6
7	2H	104	GLU	2.6
32	2a	1129	C	2.6
5	2F	6	VAL	2.6
7	2H	156	ALA	2.6
33	2b	136	VAL	2.6
34	2c	86	VAL	2.6
45	1n	18	VAL	2.6
34	2c	177	THR	2.6
51	2t	77	ALA	2.6
5	2F	16	GLY	2.6
53	2v	15	A	2.6
57	1y	51	U	2.6
1	1A	2163	C	2.6
32	1a	150	C	2.6
32	2a	980	C	2.6
7	2H	52	VAL	2.6
7	2H	115	VAL	2.6
7	2H	150	ALA	2.6
44	2m	38	GLY	2.6
26	14	52	THR	2.6
1	2A	271(K)	U	2.6
1	2A	880	G	2.6

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Mol	Chain	Res	Type	RSRZ
21	2Z	93	ASP	2.6
32	1a	1042	G	2.6
32	2a	1182	G	2.6
34	2c	178	LEU	2.6
34	2c	190	ARG	2.6
39	2h	122	ARG	2.6
52	2u	15	ARG	2.6
57	1y	50	U	2.6
45	1n	14	PRO	2.6
1	2A	363(A)	A	2.6
32	2a	1357	A	2.6
53	2v	23	A	2.6
1	2A	2804	C	2.6
8	2I	64	GLU	2.6
38	2g	31	MET	2.6
20	2Y	42	VAL	2.6
36	2e	132	ALA	2.6
38	2g	7	ALA	2.6
45	2n	45	ARG	2.6
48	2q	9	VAL	2.6
51	1t	89	ARG	2.6
41	1j	41	PRO	2.6
45	1n	61	TRP	2.6
47	2p	59	TRP	2.6
1	2A	1533	G	2.6
33	2b	126	GLU	2.6
32	2a	101	A	2.6
32	2a	1014	A	2.6
1	1A	2183	C	2.6
33	1b	216	SER	2.6
40	2i	100	GLY	2.6
7	2H	95	ARG	2.6
51	2t	40	ALA	2.6
14	2S	54	LEU	2.6
47	2p	74	LEU	2.6
48	2q	74	LEU	2.6
32	1a	170	U	2.6
33	1b	105	PHE	2.6
7	2H	78	GLY	2.6
11	2P	93	GLY	2.6
32	1a	161	A	2.6
32	2a	93	G	2.6

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Mol	Chain	Res	Type	RSRZ
33	2b	124	SER	2.6
52	2u	11	GLY	2.6
7	2H	18	GLU	2.6
33	1b	188	ALA	2.5
51	1t	76	ALA	2.5
57	2y	49	C	2.6
38	1g	80	VAL	2.5
40	1i	27	THR	2.5
33	2b	139	LYS	2.5
40	2i	75	ASP	2.5
41	2j	93	GLY	2.5
32	1a	220	G	2.5
33	2b	33	TYR	2.5
33	1b	34	ALA	2.5
57	1y	10	G	2.5
1	2A	1118	C	2.5
32	1a	848	C	2.5
32	1a	1038	C	2.5
40	1i	103	THR	2.5
33	1b	165	VAL	2.5
41	2j	39	PRO	2.5
34	2c	91	LEU	2.5
33	2b	39	ILE	2.5
7	2H	159	GLU	2.5
1	2A	900	A	2.5
14	2S	51	ALA	2.5
32	1a	1531	A	2.5
51	1t	59	ALA	2.5
1	1A	2124	G	2.5
8	2I	123	LEU	2.5
41	1j	85	LEU	2.5
48	2q	91	ARG	2.5
32	1a	479	C	2.5
32	2a	98	G	2.5
32	2a	470	C	2.5
35	2d	180	GLY	2.5
7	2H	145	ALA	2.5
33	2b	168	THR	2.5
44	2m	97	PRO	2.5
48	1q	28	PRO	2.5
51	2t	12	ALA	2.5
26	24	32	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
11	2P	148	LEU	2.5
40	2i	11	LYS	2.5
49	1r	86	VAL	2.5
53	2v	14	A	2.5
1	1A	2138	C	2.5
1	2A	2111	C	2.5
32	1a	1352	C	2.5
57	1y	43	C	2.5
20	2Y	44	ILE	2.5
32	2a	78	G	2.5
33	2b	185	ILE	2.5
41	2j	38	ILE	2.5
45	2n	7	ILE	2.5
7	2H	10	PRO	2.5
7	2H	146	ALA	2.5
29	27	45	ALA	2.5
6	2G	166	ASP	2.5
41	1j	100	THR	2.5
34	2c	43	LEU	2.5
41	2j	10	GLY	2.5
1	1A	1078	U	2.5
1	1A	1847	A	2.5
54	2w	47	U	2.5
26	24	48	ARG	2.5
32	2a	1113	C	2.5
41	2j	21	GLN	2.5
1	1A	1058	G	2.5
1	1A	1176	G	2.5
1	2A	2190	G	2.5
4	2E	31	CYS	2.5
52	2u	5	ASP	2.5
19	2X	3	THR	2.5
6	1G	146	TYR	2.5
29	27	46	VAL	2.5
51	1t	13	LEU	2.5
12	1Q	59	ARG	2.5
21	1Z	153	SER	2.5
32	2a	997	U	2.5
40	2i	18	PHE	2.5
1	1A	2177	C	2.5
32	1a	1027	C	2.5
32	2a	1037	C	2.5

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Mol	Chain	Res	Type	RSRZ
7	2H	96	ALA	2.5
8	2I	137	PRO	2.5
41	1j	16	LEU	2.4
34	1c	45	LYS	2.4
44	2m	87	TYR	2.4
1	1A	1069	A	2.4
32	1a	218	C	2.4
32	1a	457	C	2.4
36	2e	73	ASN	2.4
40	2i	89	ASN	2.4
54	2w	42	C	2.4
26	24	52	THR	2.4
33	1b	75	LYS	2.4
19	2X	95	LEU	2.4
32	2a	976	G	2.4
32	2a	1355	G	2.4
32	2a	1371	G	2.4
51	2t	72	LEU	2.4
32	2a	4	U	2.4
57	1y	66	U	2.4
6	2G	49	ASP	2.4
33	2b	80	ILE	2.4
40	2i	37	PHE	2.4
41	1j	98	ILE	2.4
21	2Z	4	ARG	2.4
32	1a	143	A	2.4
57	2y	7	A	2.4
32	2a	1045	C	2.4
44	2m	42	ALA	2.4
57	2y	72	C	2.4
7	2H	171	LEU	2.4
34	1c	87	LEU	2.4
41	2j	71	LEU	2.4
40	1i	26	VAL	2.4
47	2p	20	VAL	2.4
48	2q	85	VAL	2.4
54	1w	69	G	2.4
36	2e	13	ILE	2.4
5	1F	131	GLY	2.4
11	1P	44	GLY	2.4
38	2g	82	GLY	2.4
7	2H	29	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
32	2a	175	C	2.4
32	2a	1445	C	2.4
57	1y	68	C	2.4
39	1h	39	LEU	2.4
42	2k	98	LEU	2.4
40	2i	32	ASP	2.4
33	1b	81	VAL	2.4
33	2b	110	GLN	2.4
39	1h	43	GLY	2.4
40	2i	23	ASN	2.4
1	2A	882	G	2.4
32	2a	1293	G	2.4
1	1A	529	A	2.4
1	1A	2137	C	2.4
21	1Z	80	ARG	2.4
32	2a	1179	A	2.4
33	1b	124	SER	2.4
39	2h	103	VAL	2.4
51	1t	88	VAL	2.4
26	24	64	GLY	2.4
21	2Z	1	MET	2.4
51	1t	12	ALA	2.4
1	1A	2807	G	2.4
1	2A	2184	G	2.4
32	2a	1138	G	2.4
7	2H	63	SER	2.4
11	2P	22	GLY	2.4
22	20	65	GLY	2.4
32	1a	72	C	2.4
32	1a	134	A	2.4
33	1b	19	HIS	2.4
39	1h	67	PRO	2.4
40	2i	42	ARG	2.4
8	2I	58	LEU	2.4
10	2O	108	GLU	2.4
21	2Z	11	GLU	2.4
28	26	42	TRP	2.4
1	1A	2802	G	2.3
1	1A	1080	C	2.3
1	1A	1094	U	2.3
7	2H	4	ILE	2.3
20	2Y	56	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
40	1i	21	PRO	2.3
34	1c	83	ARG	2.3
34	2c	8	ILE	2.3
35	2d	134	ASP	2.3
41	1j	29	ARG	2.3
51	2t	25	ARG	2.3
26	24	67	TYR	2.3
7	2H	46	GLU	2.3
41	2j	27	ALA	2.3
26	24	27	THR	2.3
8	2I	72	LEU	2.3
24	22	32	LEU	2.3
1	1A	1068	G	2.3
3	2D	51	VAL	2.3
21	1Z	167	PRO	2.3
57	1y	33	U	2.3
1	1A	2107	C	2.3
32	2a	161	A	2.3
40	1i	55	ALA	2.3
40	2i	13	ALA	2.3
51	2t	38	LYS	2.3
21	2Z	16	SER	2.3
11	2P	109	GLY	2.3
5	1F	20	LEU	2.3
21	2Z	70	LEU	2.3
33	2b	187	LEU	2.3
38	2g	101	LEU	2.3
41	1j	46	ARG	2.3
5	2F	96	ASP	2.3
33	2b	219	VAL	2.3
32	2a	1057	G	2.3
32	2a	1133	G	2.3
57	1y	65	G	2.3
2	2B	59	A	2.3
8	2I	89	TYR	2.3
33	2b	204	ASN	2.3
40	1i	88	TYR	2.3
40	2i	126	SER	2.3
41	2j	26	ALA	2.3
38	2g	34	GLY	2.3
33	2b	36	ARG	2.3
33	2b	215	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
40	2i	10	ARG	2.3
45	2n	29	ARG	2.3
16	2U	2	PRO	2.3
21	1Z	139	VAL	2.3
46	2o	60	VAL	2.3
50	2s	11	VAL	2.3
1	1A	2189	U	2.3
6	2G	39	ILE	2.3
38	2g	27	ILE	2.3
1	1A	886	C	2.3
40	1i	52	ALA	2.3
44	2m	119	GLY	2.3
1	2A	881	G	2.3
32	2a	105	G	2.3
40	1i	113	LYS	2.3
40	2i	38	GLN	2.3
44	2m	122	LYS	2.3
51	2t	29	LYS	2.3
48	2q	30	PRO	2.3
8	2I	144	VAL	2.3
26	14	50	VAL	2.3
1	1A	2150	U	2.3
8	2I	41	GLU	2.3
52	1u	14	TRP	2.3
45	1n	55	GLY	2.3
48	2q	54	GLY	2.3
51	2t	69	GLY	2.3
6	2G	61	ALA	2.3
44	2m	121	LYS	2.3
38	2g	56	GLN	2.3
32	2a	1326	C	2.3
21	2Z	91	LEU	2.3
21	2Z	157	LEU	2.3
1	1A	1055	G	2.3
1	1A	2100	G	2.3
1	1A	2104	G	2.3
7	2H	168	PRO	2.3
39	2h	37	ARG	2.3
48	2q	21	VAL	2.3
51	2t	8	ARG	2.3
31	29	13	LYS	2.3
42	2k	94	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
22	10	43	THR	2.3
40	1i	125	TYR	2.3
1	2A	2188	C	2.3
26	24	18	CYS	2.3
31	29	11	CYS	2.3
32	2a	422	C	2.3
32	2a	1362	C	2.3
34	2c	196	LEU	2.3
35	2d	196	LEU	2.3
45	1n	11	LYS	2.2
1	2A	2792	G	2.2
32	2a	1273	G	2.2
57	1y	29	G	2.2
12	2Q	33	GLY	2.2
32	1a	1012	U	2.2
32	2a	1136	U	2.2
34	1c	8	ILE	2.2
51	2t	55	ILE	2.2
7	2H	34	GLU	2.2
8	1I	86	THR	2.2
28	26	12	GLU	2.2
44	2m	64	TRP	2.2
21	1Z	70	LEU	2.2
33	2b	111	ARG	2.2
38	2g	58	PRO	2.2
32	2a	1354	C	2.2
57	2y	41	C	2.2
28	26	43	CYS	2.2
5	2F	114	VAL	2.2
32	2a	1252	A	2.2
32	2a	1324	A	2.2
1	2A	2102	U	2.2
32	2a	220	G	2.2
26	14	49	PHE	2.2
42	2k	65	ALA	2.2
47	1p	22	THR	2.2
50	2s	57	HIS	2.2
49	1r	42	ARG	2.2
51	1t	17	ARG	2.2
51	1t	24	LEU	2.2
11	2P	97	PRO	2.2
33	2b	31	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
21	2Z	145	GLU	2.2
32	1a	470	C	2.2
33	1b	128	GLU	2.2
1	2A	6	A	2.2
1	2A	2176	A	2.2
20	2Y	54	LYS	2.2
32	1a	90	U	2.2
32	1a	149	A	2.2
21	2Z	172	ALA	2.2
26	24	68	ARG	2.2
51	1t	79	ARG	2.2
44	1m	103	THR	2.2
1	2A	363	G	2.2
32	1a	98	G	2.2
32	2a	77	G	2.2
32	2a	1011	G	2.2
4	2E	63	LEU	2.2
21	1Z	163	LEU	2.2
40	2i	98	PRO	2.2
47	1p	59	TRP	2.2
40	2i	125	TYR	2.2
44	2m	120	LYS	2.2
1	1A	2804	C	2.2
1	2A	2185	C	2.2
32	1a	91	C	2.2
32	2a	92	C	2.2
32	2a	1018	C	2.2
32	2a	1148	U	2.2
6	2G	145	THR	2.2
32	2a	1004	A	2.2
32	2a	1092	A	2.2
51	1t	94	ALA	2.2
41	1j	21	GLN	2.2
33	1b	61	LEU	2.2
40	2i	85	LEU	2.2
1	2A	1170	G	2.2
32	2a	61	G	2.2
32	2a	1368	G	2.2
51	1t	22	ARG	2.2
48	2q	12	SER	2.2
12	2Q	109	VAL	2.2
33	1b	15	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
50	2s	51	VAL	2.2
1	1A	885	C	2.2
1	2A	2105	C	2.2
14	2S	84	GLN	2.2
16	2U	107	ALA	2.2
32	2a	1161	C	2.2
33	2b	45	GLN	2.2
34	2c	44	GLU	2.2
45	2n	16	PHE	2.2
19	1X	94	GLY	2.2
24	22	42	GLY	2.2
26	24	62	ARG	2.2
51	2t	22	ARG	2.2
1	1A	652(C)	G	2.2
7	2H	85	LYS	2.2
21	2Z	128	VAL	2.2
51	1t	40	ALA	2.2
1	1A	1075	C	2.2
1	1A	1079	C	2.2
11	2P	96	THR	2.2
21	2Z	133	ILE	2.2
32	2a	1128	C	2.2
41	2j	12	ASP	2.2
26	14	48	ARG	2.2
45	2n	19	ARG	2.2
1	1A	1077	A	2.2
21	2Z	38	TYR	2.1
1	1A	1171	G	2.1
19	2X	91	ALA	2.1
32	2a	1143	G	2.1
34	2c	195	VAL	2.1
38	1g	25	ALA	2.1
51	2t	67	ALA	2.1
54	2w	29	G	2.1
6	2G	65	GLY	2.1
40	2i	64	THR	2.1
44	2m	20	THR	2.1
1	2A	1043	C	2.1
32	1a	1161	C	2.1
39	2h	33	GLU	2.1
33	2b	118	LEU	2.1
39	2h	112	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
41	2j	85	LEU	2.1
41	2j	90	LEU	2.1
49	1r	31	LEU	2.1
51	2t	62	LEU	2.1
50	2s	28	LYS	2.1
1	1A	2134	A	2.1
32	1a	344	A	2.1
32	1a	1180	A	2.1
33	1b	78	GLN	2.1
40	2i	92	TYR	2.1
1	1A	2122	U	2.1
33	1b	93	VAL	2.1
33	2b	173	ALA	2.1
41	1j	20	ALA	2.1
49	2r	86	VAL	2.1
49	2r	47	THR	2.1
1	2A	295	G	2.1
16	2U	62	ILE	2.1
33	1b	208	ILE	2.1
33	2b	208	ILE	2.1
12	2Q	17	LEU	2.1
33	2b	95	GLN	2.1
32	2a	271	C	2.1
57	1y	25	C	2.1
57	2y	13	C	2.1
21	1Z	149	SER	2.1
1	1A	878	A	2.1
1	1A	2176	A	2.1
40	1i	20	ARG	2.1
11	1P	98	GLU	2.1
57	1y	31	A	2.1
6	2G	24	GLY	2.1
36	1e	34	VAL	2.1
38	2g	44	TYR	2.1
38	2g	55	GLY	2.1
45	1n	51	GLY	2.1
1	1A	1083	U	2.1
5	2F	189	THR	2.1
33	2b	54	THR	2.1
34	2c	165	THR	2.1
41	2j	87	THR	2.1
35	1d	70	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
51	1t	18	GLN	2.1
32	1a	166	G	2.1
1	1A	174	C	2.1
15	2T	128	GLU	2.1
47	1p	61	SER	2.1
32	1a	849	C	2.1
32	1a	1118	C	2.1
32	2a	840	C	2.1
54	2w	2	C	2.1
46	2o	58	MET	2.1
48	1q	8	GLY	2.1
1	2A	228	A	2.1
15	2T	126	ALA	2.1
30	28	17	THR	2.1
32	1a	203	U	2.1
32	2a	1000	U	2.1
33	2b	171	ALA	2.1
41	2j	18	ALA	2.1
34	2c	95	THR	2.1
41	2j	41	PRO	2.1
40	2i	74	ILE	2.1
7	2H	101	ARG	2.1
33	2b	205	ASP	2.1
38	2g	16	LEU	2.1
38	2g	26	PHE	2.1
38	2g	32	ARG	2.1
20	1Y	52	SER	2.1
40	2i	113	LYS	2.1
48	1q	66	SER	2.1
48	2q	66	SER	2.1
34	2c	102	ASN	2.1
19	1X	24	GLY	2.1
32	2a	1385	G	2.1
36	2e	85	GLY	2.1
47	1p	1	MET	2.1
48	1q	82	MET	2.1
12	2Q	32	TYR	2.1
38	2g	4	ARG	2.1
14	2S	32	LEU	2.1
21	2Z	18	LEU	2.1
22	20	60	PHE	2.1
41	1j	73	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
40	2i	50	LEU	2.1
48	1q	89	LEU	2.1
48	2q	98	LEU	2.1
34	1c	25	GLY	2.1
34	2c	41	GLY	2.1
1	1A	652(T)	C	2.1
8	2I	73	GLU	2.1
33	1b	48	MET	2.1
3	1D	191	ALA	2.1
19	2X	42	ALA	2.1
29	27	47	ARG	2.1
32	1a	1010	G	2.1
35	1d	111	ALA	2.1
38	2g	78	ARG	2.1
49	1r	73	ALA	2.1
1	2A	2118	U	2.1
48	2q	23	VAL	2.1
21	2Z	8	TYR	2.1
41	2j	23	ILE	2.1
38	1g	12	LEU	2.1
5	2F	200	GLU	2.1
26	24	39	CYS	2.1
33	2b	227	GLY	2.1
34	2c	205	GLY	2.1
40	2i	24	GLY	2.1
33	1b	24	TRP	2.1
38	2g	41	ARG	2.1
40	2i	128	ARG	2.1
45	2n	15	LYS	2.1
1	2A	2870	C	2.0
21	2Z	21	ALA	2.0
32	1a	165	C	2.0
32	1a	175	C	2.0
40	1i	15	ALA	2.0
41	2j	73	ASP	2.0
42	2k	74	ALA	2.0
11	2P	58	THR	2.0
40	1i	65	VAL	2.0
32	2a	838	G	2.0
51	2t	16	HIS	2.0
47	1p	17	TYR	2.0
57	2y	27	G	2.0

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Mol	Chain	Res	Type	RSRZ
31	29	17	ILE	2.0
34	2c	134	ILE	2.0
44	2m	48	LEU	2.0
3	2D	223	GLY	2.0
54	1w	73	A	2.0
57	1y	7	A	2.0
46	2o	10	LYS	2.0
41	1j	45	ARG	2.0
33	2b	29	ALA	2.0
38	2g	2	ALA	2.0
41	1j	39	PRO	2.0
1	1A	1963	U	2.0
15	2T	59	THR	2.0
20	2Y	24	VAL	2.0
32	2a	848	C	2.0
40	1i	126	SER	2.0
42	1k	79	SER	2.0
21	2Z	20	ARG	2.0
41	1j	11	PHE	2.0
45	2n	41	ARG	2.0
2	2B	56	G	2.0
32	1a	183	G	2.0
1	1A	1070	A	2.0
32	2a	1279	A	2.0
36	1e	148	VAL	2.0
40	1i	89	ASN	2.0
47	1p	62	VAL	2.0
5	1F	17	ARG	2.0
33	1b	185	ILE	2.0
40	2i	81	ILE	2.0
57	2y	4	C	2.0
47	2p	32	TYR	2.0
40	2i	110	GLU	2.0
51	1t	64	ASP	2.0
1	2A	100	G	2.0
32	1a	1276	G	2.0
32	2a	1285	A	2.0
57	2y	22	G	2.0
33	2b	183	PRO	2.0
41	2j	91	PRO	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	4SU	2y	8	20/21	0.63	0.30	76,87,92,101	0
57	MIA	2y	37	22/30	0.64	0.49	68,77,91,101	0
57	PSU	2y	32	20/21	0.66	0.32	70,77,83,86	0
57	G7M	2y	46	24/25	0.67	0.30	73,82,88,90	0
54	G7M	2w	46	24/25	0.67	0.23	61,76,89,101	0
57	5MU	2y	54	21/22	0.68	0.36	70,78,87,101	0
57	4SU	1y	8	20/21	0.69	0.28	76,80,87,101	0
57	G7M	1y	46	24/25	0.69	0.28	75,80,85,93	0
57	PSU	2y	39	20/21	0.71	0.43	71,79,88,94	0
57	MIA	1y	37	22/30	0.71	0.43	72,78,86,95	0
57	PSU	1y	55	20/21	0.72	0.49	76,81,89,94	0
57	PSU	1y	39	20/21	0.76	0.35	71,77,86,86	0
57	PSU	2y	55	20/21	0.77	0.43	75,80,90,90	0
57	5MU	1y	54	21/22	0.79	0.36	72,77,84,87	0
54	G7M	1w	46	24/25	0.79	0.20	59,69,79,99	0
57	PSU	1y	32	20/21	0.79	0.31	67,75,84,84	0
54	MIA	2w	37	25/30	0.84	0.24	56,64,67,85	0
54	4SU	2w	8	20/21	0.85	0.18	70,75,81,88	0
54	4SU	1w	8	20/21	0.86	0.17	68,74,81,81	0
32	2MG	2a	1207	24/25	0.86	0.22	56,67,72,76	0
54	PSU	2w	32	20/21	0.86	0.26	57,63,75,78	0
54	PSU	2w	55	20/21	0.87	0.19	58,70,73,73	0
54	PSU	1w	55	20/21	0.88	0.19	42,60,65,66	0
32	M2G	2a	966	25/26	0.88	0.23	53,56,64,73	0
54	5MU	2w	54	21/22	0.89	0.16	50,64,66,69	0
55	5MU	2x	54	21/22	0.89	0.21	58,66,73,77	0
43	0TD	2l	92	10/11	0.89	0.18	49,51,56,67	0
55	PSU	2x	55	20/21	0.90	0.19	59,65,72,74	0
55	4SU	2x	8	20/21	0.90	0.17	58,63,66,68	0
54	MIA	1w	37	29/30	0.90	0.22	33,45,54,82	0
43	0TD	1l	92	10/11	0.90	0.15	39,44,45,60	0
54	PSU	2w	39	20/21	0.90	0.24	57,65,71,72	0
55	5MU	1x	54	21/22	0.91	0.17	53,58,66,73	0
32	G7M	2a	527	24/25	0.91	0.18	43,56,61,65	0
54	PSU	1w	39	20/21	0.92	0.21	37,55,60,68	0
55	5MC	2x	32	21/22	0.92	0.19	52,58,64,68	0
1	OMU	2A	2552	21/22	0.92	0.23	36,42,46,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	PSU	1w	32	20/21	0.92	0.17	49,55,62,62	0
32	MA6	2a	1519	24/25	0.92	0.27	44,53,59,62	0
55	PSU	1x	55	20/21	0.92	0.22	48,54,60,65	0
1	5MU	2A	1915	21/22	0.92	0.18	44,55,61,62	0
1	OMC	2A	1920	21/22	0.93	0.20	45,53,55,56	0
32	5MC	2a	967	21/22	0.93	0.19	51,57,60,65	0
55	4SU	1x	8	20/21	0.93	0.17	49,58,65,68	0
32	5MC	2a	1400	21/22	0.93	0.21	52,60,64,68	0
32	4OC	2a	1402	22/23	0.93	0.18	46,49,54,56	0
32	MA6	2a	1518	24/25	0.93	0.20	42,50,55,58	0
32	PSU	2a	516	20/21	0.93	0.17	54,62,66,67	0
1	PSU	2A	1917	20/21	0.93	0.17	48,53,59,64	0
55	5MC	1x	32	21/22	0.94	0.18	34,45,50,62	0
32	2MG	1a	1207	24/25	0.94	0.16	49,57,61,66	0
32	5MC	1a	1400	21/22	0.94	0.17	36,45,48,50	0
54	5MU	1w	54	21/22	0.94	0.17	40,54,60,62	0
32	4OC	1a	1402	22/23	0.94	0.19	33,37,42,46	0
1	5MU	1A	1915	21/22	0.94	0.19	36,42,46,47	0
32	M2G	1a	966	25/26	0.94	0.19	41,48,52,53	0
32	5MC	1a	967	21/22	0.95	0.19	43,48,53,56	0
32	PSU	1a	516	20/21	0.95	0.17	40,51,55,56	0
55	8AN	2x	76	22/23	0.95	0.24	31,35,41,46	0
32	G7M	1a	527	24/25	0.95	0.20	33,42,46,52	0
1	5MC	2A	1942	21/22	0.95	0.22	43,50,56,57	0
32	5MC	2a	1404	21/22	0.95	0.20	40,46,50,63	0
32	5MC	2a	1407	21/22	0.95	0.22	42,45,51,53	0
1	5MC	2A	1962	21/22	0.95	0.22	32,40,49,62	0
1	PSU	1A	1917	20/21	0.95	0.17	31,40,44,45	0
32	5MC	1a	1404	21/22	0.95	0.20	31,40,45,46	0
32	MA6	1a	1519	24/25	0.95	0.20	34,40,43,51	0
1	PSU	2A	1911	20/21	0.95	0.17	45,53,56,57	0
54	F3N	2w	76	33/34	0.95	0.23	27,35,42,46	0
1	OMG	2A	2251	24/25	0.96	0.22	30,35,39,41	0
55	8AN	1x	76	22/23	0.96	0.22	14,19,24,25	0
32	UR3	2a	1498	21/22	0.96	0.20	43,49,55,60	0
1	PSU	2A	2605	20/21	0.96	0.20	25,32,37,38	0
1	PSU	1A	1911	20/21	0.96	0.19	26,40,45,47	0
1	OMC	1A	1920	21/22	0.96	0.21	30,37,42,44	0
1	2MA	1A	2503	23/24	0.96	0.22	12,16,19,21	0
1	PSU	1A	2605	20/21	0.96	0.21	18,23,28,28	0
1	5MU	2A	1939	21/22	0.96	0.22	30,37,41,45	0
32	5MC	1a	1407	21/22	0.96	0.21	31,36,40,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	UR3	1a	1498	21/22	0.96	0.21	33,38,41,43	0
1	5MU	1A	1939	21/22	0.97	0.22	21,24,30,31	0
1	5MC	1A	1942	21/22	0.97	0.20	23,34,40,54	0
1	5MC	1A	1962	21/22	0.97	0.20	27,31,35,37	0
54	F3N	1w	76	33/34	0.97	0.23	13,17,21,24	0
32	MA6	1a	1518	24/25	0.97	0.21	33,39,44,45	0
1	OMU	1A	2552	21/22	0.98	0.20	16,23,27,29	0
1	2MA	2A	2503	23/24	0.98	0.20	28,35,39,42	0
1	OMG	1A	2251	24/25	0.98	0.22	17,22,24,25	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3951	1/1	0.10	0.10	53,53,53,53	0
58	MG	2a	1758	1/1	0.29	0.16	78,78,78,78	0
58	MG	2v	103	1/1	0.33	0.18	70,70,70,70	0
58	MG	1B	216	1/1	0.34	0.12	49,49,49,49	0
58	MG	2A	3362	1/1	0.35	0.18	68,68,68,68	0
58	MG	1A	3659	1/1	0.40	0.18	30,30,30,30	0
58	MG	1A	4072	1/1	0.40	0.26	58,58,58,58	0
58	MG	1A	3845	1/1	0.40	0.22	60,60,60,60	0
58	MG	2A	3257	1/1	0.43	0.26	61,61,61,61	0
58	MG	1A	3958	1/1	0.43	0.09	39,39,39,39	0
58	MG	10	105	1/1	0.45	0.33	58,58,58,58	0
58	MG	1a	1790	1/1	0.47	0.15	62,62,62,62	0
58	MG	1A	3802	1/1	0.48	0.17	73,73,73,73	0
58	MG	2A	3511	1/1	0.52	0.23	46,46,46,46	0
58	MG	1A	3186	1/1	0.52	0.11	62,62,62,62	0
58	MG	1A	4006	1/1	0.52	0.20	40,40,40,40	0
58	MG	2A	3528	1/1	0.53	0.22	62,62,62,62	0
58	MG	2a	1748	1/1	0.53	0.17	78,78,78,78	0
58	MG	1A	3859	1/1	0.53	0.24	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3336	1/1	0.53	0.23	66,66,66,66	0
58	MG	2A	3839	1/1	0.54	0.16	57,57,57,57	0
58	MG	2a	1774	1/1	0.54	0.10	61,61,61,61	0
58	MG	2A	3480	1/1	0.54	0.39	70,70,70,70	0
58	MG	1A	3865	1/1	0.56	0.27	68,68,68,68	0
58	MG	1A	3998	1/1	0.56	0.19	29,29,29,29	0
58	MG	2A	3265	1/1	0.56	0.26	65,65,65,65	0
58	MG	2a	1635	1/1	0.56	0.15	66,66,66,66	0
58	MG	1A	4076	1/1	0.57	0.10	54,54,54,54	0
58	MG	1a	1629	1/1	0.59	0.17	52,52,52,52	0
58	MG	1A	3959	1/1	0.60	0.09	56,56,56,56	0
58	MG	1A	3436	1/1	0.60	0.37	50,50,50,50	0
58	MG	1A	3307	1/1	0.61	0.32	36,36,36,36	0
58	MG	1A	3566	1/1	0.61	0.12	71,71,71,71	0
58	MG	1a	1800	1/1	0.61	0.13	61,61,61,61	0
58	MG	2a	1739	1/1	0.61	0.16	56,56,56,56	0
58	MG	2w	103	1/1	0.61	0.36	63,63,63,63	0
58	MG	1a	1811	1/1	0.62	0.17	61,61,61,61	0
58	MG	1A	3655	1/1	0.62	0.13	64,64,64,64	0
58	MG	2A	3050	1/1	0.63	0.19	67,67,67,67	0
58	MG	2a	1627	1/1	0.63	0.18	65,65,65,65	0
58	MG	1a	1672	1/1	0.63	0.19	60,60,60,60	0
58	MG	2A	3401	1/1	0.64	0.17	65,65,65,65	0
58	MG	2a	1660	1/1	0.64	0.24	52,52,52,52	0
58	MG	1A	4040	1/1	0.64	0.13	38,38,38,38	0
58	MG	1A	4045	1/1	0.64	0.13	40,40,40,40	0
58	MG	1A	3095	1/1	0.65	0.15	55,55,55,55	0
58	MG	2a	1775	1/1	0.65	0.18	53,53,53,53	0
58	MG	2a	1725	1/1	0.66	0.12	59,59,59,59	0
58	MG	2A	3262	1/1	0.66	0.26	59,59,59,59	0
58	MG	1a	1803	1/1	0.66	0.14	57,57,57,57	0
58	MG	1B	231	1/1	0.66	0.17	61,61,61,61	0
58	MG	1A	4070	1/1	0.67	0.17	56,56,56,56	0
58	MG	2A	3704	1/1	0.67	0.20	60,60,60,60	0
58	MG	2A	3786	1/1	0.67	0.12	63,63,63,63	0
58	MG	2a	1833	1/1	0.67	0.16	63,63,63,63	0
58	MG	1a	1743	1/1	0.67	0.17	77,77,77,77	0
58	MG	1O	201	1/1	0.67	0.26	58,58,58,58	0
58	MG	2A	3342	1/1	0.68	0.17	69,69,69,69	0
58	MG	1A	3637	1/1	0.68	0.11	61,61,61,61	0
58	MG	2A	3065	1/1	0.68	0.23	57,57,57,57	0
58	MG	1A	4002	1/1	0.68	0.12	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3798	1/1	0.68	0.09	41,41,41,41	0
58	MG	1A	4030	1/1	0.68	0.12	52,52,52,52	0
58	MG	2A	3596	1/1	0.68	0.11	60,60,60,60	0
58	MG	2A	3683	1/1	0.68	0.18	60,60,60,60	0
58	MG	2A	3289	1/1	0.68	0.20	61,61,61,61	0
58	MG	2a	1796	1/1	0.68	0.10	54,54,54,54	0
58	MG	2A	3322	1/1	0.68	0.24	62,62,62,62	0
58	MG	1A	3335	1/1	0.68	0.26	50,50,50,50	0
58	MG	2T	202	1/1	0.68	0.16	70,70,70,70	0
58	MG	2A	3805	1/1	0.69	0.30	54,54,54,54	0
58	MG	1A	3992	1/1	0.69	0.16	60,60,60,60	0
58	MG	1A	3995	1/1	0.69	0.22	38,38,38,38	0
58	MG	1A	4031	1/1	0.69	0.11	55,55,55,55	0
58	MG	1A	3884	1/1	0.69	0.10	41,41,41,41	0
58	MG	2A	3070	1/1	0.69	0.18	49,49,49,49	0
58	MG	1A	3002	1/1	0.69	0.26	56,56,56,56	0
58	MG	1A	4046	1/1	0.69	0.17	49,49,49,49	0
58	MG	2A	3291	1/1	0.70	0.25	58,58,58,58	0
58	MG	1A	3955	1/1	0.70	0.07	45,45,45,45	0
58	MG	2A	3838	1/1	0.70	0.14	63,63,63,63	0
58	MG	2A	3253	1/1	0.70	0.26	62,62,62,62	0
58	MG	1A	4041	1/1	0.70	0.10	50,50,50,50	0
58	MG	2A	3706	1/1	0.70	0.22	52,52,52,52	0
58	MG	2a	1666	1/1	0.71	0.12	65,65,65,65	0
58	MG	2a	1680	1/1	0.71	0.14	50,50,50,50	0
58	MG	1A	3987	1/1	0.71	0.10	52,52,52,52	0
58	MG	2A	3273	1/1	0.71	0.16	65,65,65,65	0
58	MG	1a	1699	1/1	0.71	0.16	57,57,57,57	0
58	MG	2A	3073	1/1	0.71	0.20	54,54,54,54	0
58	MG	1a	1708	1/1	0.72	0.31	55,55,55,55	0
58	MG	2A	3744	1/1	0.72	0.33	66,66,66,66	0
58	MG	1B	238	1/1	0.72	0.13	35,35,35,35	0
58	MG	2A	3173	1/1	0.72	0.20	66,66,66,66	0
58	MG	1w	109	1/1	0.72	0.14	72,72,72,72	0
58	MG	2A	3543	1/1	0.72	0.21	56,56,56,56	0
58	MG	2A	3848	1/1	0.72	0.28	38,38,38,38	0
58	MG	2A	3041	1/1	0.72	0.36	49,49,49,49	0
58	MG	2a	1614	1/1	0.72	0.11	54,54,54,54	0
58	MG	1A	3811	1/1	0.72	0.13	36,36,36,36	0
58	MG	2a	1628	1/1	0.72	0.26	64,64,64,64	0
58	MG	1A	3261	1/1	0.72	0.25	36,36,36,36	0
58	MG	2a	1640	1/1	0.72	0.26	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3185	1/1	0.73	0.13	52,52,52,52	0
58	MG	1a	1774	1/1	0.73	0.15	63,63,63,63	0
58	MG	1v	101	1/1	0.73	0.14	60,60,60,60	0
58	MG	1A	3749	1/1	0.73	0.12	47,47,47,47	0
58	MG	2A	3315	1/1	0.73	0.22	57,57,57,57	0
58	MG	2A	3263	1/1	0.73	0.30	40,40,40,40	0
58	MG	2a	1751	1/1	0.73	0.10	73,73,73,73	0
58	MG	2A	3823	1/1	0.74	0.15	66,66,66,66	0
58	MG	2A	3864	1/1	0.74	0.47	61,61,61,61	0
58	MG	1A	3312	1/1	0.74	0.17	57,57,57,57	0
58	MG	2j	201	1/1	0.74	0.24	65,65,65,65	0
58	MG	2a	1714	1/1	0.74	0.15	66,66,66,66	0
58	MG	1A	3964	1/1	0.74	0.10	49,49,49,49	0
58	MG	1A	3800	1/1	0.75	0.10	42,42,42,42	0
58	MG	1a	1753	1/1	0.75	0.13	45,45,45,45	0
58	MG	2A	3745	1/1	0.75	0.19	44,44,44,44	0
58	MG	1a	1770	1/1	0.75	0.09	68,68,68,68	0
58	MG	2A	3192	1/1	0.75	0.27	51,51,51,51	0
58	MG	1a	1773	1/1	0.75	0.07	57,57,57,57	0
58	MG	2a	1646	1/1	0.75	0.19	59,59,59,59	0
58	MG	2A	3612	1/1	0.75	0.11	54,54,54,54	0
58	MG	2a	1661	1/1	0.75	0.24	52,52,52,52	0
58	MG	1A	3434	1/1	0.75	0.33	45,45,45,45	0
58	MG	2A	3698	1/1	0.75	0.16	53,53,53,53	0
58	MG	2A	3404	1/1	0.75	0.11	53,53,53,53	0
58	MG	2A	3666	1/1	0.76	0.14	57,57,57,57	0
58	MG	1a	1809	1/1	0.76	0.14	48,48,48,48	0
58	MG	2A	3688	1/1	0.76	0.15	51,51,51,51	0
58	MG	1A	3440	1/1	0.76	0.17	44,44,44,44	0
58	MG	1O	205	1/1	0.76	0.23	48,48,48,48	0
58	MG	2A	3231	1/1	0.76	0.32	38,38,38,38	0
58	MG	1A	3645	1/1	0.76	0.20	50,50,50,50	0
58	MG	2A	3024	1/1	0.76	0.26	61,61,61,61	0
58	MG	1A	3850	1/1	0.76	0.16	48,48,48,48	0
58	MG	1A	3461	1/1	0.76	0.21	52,52,52,52	0
58	MG	2A	3483	1/1	0.76	0.17	62,62,62,62	0
58	MG	1A	3258	1/1	0.76	0.16	49,49,49,49	0
58	MG	2A	3521	1/1	0.76	0.26	60,60,60,60	0
58	MG	2A	3843	1/1	0.76	0.17	41,41,41,41	0
58	MG	2A	3067	1/1	0.76	0.19	62,62,62,62	0
58	MG	1A	3873	1/1	0.76	0.09	41,41,41,41	0
58	MG	2A	3868	1/1	0.76	0.33	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1a	1732	1/1	0.76	0.15	41,41,41,41	0
58	MG	2a	1609	1/1	0.76	0.25	61,61,61,61	0
58	MG	2A	3301	1/1	0.76	0.33	67,67,67,67	0
58	MG	2A	3613	1/1	0.76	0.23	37,37,37,37	0
58	MG	2A	3844	1/1	0.77	0.39	74,74,74,74	0
58	MG	1A	4035	1/1	0.77	0.25	35,35,35,35	0
58	MG	2a	1682	1/1	0.77	0.39	58,58,58,58	0
58	MG	2a	1691	1/1	0.77	0.15	64,64,64,64	0
58	MG	1E	311	1/1	0.77	0.14	60,60,60,60	0
58	MG	1B	213	1/1	0.77	0.26	46,46,46,46	0
58	MG	2F	302	1/1	0.77	0.21	56,56,56,56	0
58	MG	2A	3709	1/1	0.77	0.25	71,71,71,71	0
58	MG	1A	4043	1/1	0.77	0.15	40,40,40,40	0
58	MG	1Z	302	1/1	0.77	0.18	62,62,62,62	0
58	MG	2A	3223	1/1	0.77	0.47	51,51,51,51	0
58	MG	2A	3803	1/1	0.77	0.14	57,57,57,57	0
58	MG	2A	3618	1/1	0.77	0.25	39,39,39,39	0
58	MG	1A	3961	1/1	0.77	0.07	53,53,53,53	0
58	MG	2A	3237	1/1	0.77	0.31	46,46,46,46	0
58	MG	1B	232	1/1	0.77	0.11	50,50,50,50	0
58	MG	2A	3689	1/1	0.77	0.32	44,44,44,44	0
58	MG	2A	3410	1/1	0.78	0.24	60,60,60,60	0
58	MG	2A	3449	1/1	0.78	0.33	56,56,56,56	0
58	MG	2A	3216	1/1	0.78	0.26	54,54,54,54	0
58	MG	2a	1747	1/1	0.78	0.16	60,60,60,60	0
58	MG	2A	3348	1/1	0.78	0.08	70,70,70,70	0
58	MG	2A	3621	1/1	0.78	0.29	47,47,47,47	0
58	MG	2A	3645	1/1	0.78	0.25	39,39,39,39	0
58	MG	1a	1736	1/1	0.78	0.13	56,56,56,56	0
58	MG	2D	307	1/1	0.78	0.24	54,54,54,54	0
58	MG	2A	3385	1/1	0.78	0.17	45,45,45,45	0
58	MG	2a	1799	1/1	0.78	0.16	61,61,61,61	0
58	MG	2T	201	1/1	0.78	0.20	59,59,59,59	0
58	MG	1a	1797	1/1	0.78	0.06	67,67,67,67	0
58	MG	2l	201	1/1	0.78	0.22	53,53,53,53	0
58	MG	1A	3787	1/1	0.78	0.16	43,43,43,43	0
58	MG	2a	1706	1/1	0.78	0.16	59,59,59,59	0
58	MG	1A	4048	1/1	0.79	0.16	35,35,35,35	0
58	MG	1A	4058	1/1	0.79	0.11	47,47,47,47	0
58	MG	2A	3757	1/1	0.79	0.17	36,36,36,36	0
58	MG	2A	3541	1/1	0.79	0.21	59,59,59,59	0
58	MG	2a	1647	1/1	0.79	0.13	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3799	1/1	0.79	0.20	63,63,63,63	0
58	MG	1a	1782	1/1	0.79	0.12	64,64,64,64	0
58	MG	2A	3594	1/1	0.79	0.15	51,51,51,51	0
58	MG	1A	3248	1/1	0.79	0.26	52,52,52,52	0
58	MG	2A	3824	1/1	0.79	0.11	41,41,41,41	0
58	MG	1a	1613	1/1	0.79	0.12	62,62,62,62	0
58	MG	1A	3851	1/1	0.79	0.16	52,52,52,52	0
58	MG	2A	3842	1/1	0.79	0.14	49,49,49,49	0
58	MG	1a	1666	1/1	0.79	0.21	57,57,57,57	0
58	MG	1A	3300	1/1	0.79	0.38	51,51,51,51	0
58	MG	1A	3457	1/1	0.79	0.21	51,51,51,51	0
58	MG	2A	3646	1/1	0.79	0.18	40,40,40,40	0
58	MG	1b	301	1/1	0.79	0.16	66,66,66,66	0
58	MG	2B	207	1/1	0.79	0.20	51,51,51,51	0
58	MG	1A	3375	1/1	0.79	0.25	47,47,47,47	0
58	MG	1A	3985	1/1	0.79	0.14	41,41,41,41	0
58	MG	1A	3717	1/1	0.79	0.23	25,25,25,25	0
58	MG	1A	3895	1/1	0.79	0.14	47,47,47,47	0
58	MG	20	102	1/1	0.79	0.16	56,56,56,56	0
58	MG	1A	3150	1/1	0.79	0.27	35,35,35,35	0
58	MG	2a	1612	1/1	0.79	0.13	66,66,66,66	0
58	MG	2l	204	1/1	0.79	0.17	49,49,49,49	0
58	MG	2q	202	1/1	0.79	0.14	57,57,57,57	0
58	MG	1A	3952	1/1	0.79	0.09	39,39,39,39	0
58	MG	2w	102	1/1	0.79	0.20	54,54,54,54	0
58	MG	2A	3274	1/1	0.79	0.18	52,52,52,52	0
58	MG	2A	3501	1/1	0.80	0.13	50,50,50,50	0
58	MG	1a	1650	1/1	0.80	0.22	42,42,42,42	0
58	MG	1A	3722	1/1	0.80	0.17	47,47,47,47	0
58	MG	1A	3501	1/1	0.80	0.18	46,46,46,46	0
58	MG	1A	3640	1/1	0.80	0.10	28,28,28,28	0
58	MG	2A	3111	1/1	0.80	0.16	39,39,39,39	0
58	MG	2A	3350	1/1	0.80	0.18	53,53,53,53	0
58	MG	1A	3667	1/1	0.80	0.20	44,44,44,44	0
58	MG	28	103	1/1	0.80	0.23	54,54,54,54	0
58	MG	1a	1610	1/1	0.80	0.12	61,61,61,61	0
58	MG	2a	1767	1/1	0.80	0.07	59,59,59,59	0
58	MG	1a	1795	1/1	0.80	0.31	64,64,64,64	0
58	MG	2A	3039	1/1	0.80	0.27	48,48,48,48	0
58	MG	2A	3809	1/1	0.80	0.13	60,60,60,60	0
58	MG	1A	3677	1/1	0.80	0.12	37,37,37,37	0
58	MG	2A	3623	1/1	0.80	0.17	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3423	1/1	0.80	0.27	37,37,37,37	0
58	MG	2A	3296	1/1	0.80	0.13	62,62,62,62	0
58	MG	1A	3567	1/1	0.80	0.30	55,55,55,55	0
58	MG	2A	3305	1/1	0.80	0.39	53,53,53,53	0
58	MG	2A	3487	1/1	0.80	0.19	54,54,54,54	0
58	MG	2A	3498	1/1	0.80	0.30	71,71,71,71	0
58	MG	2A	3856	1/1	0.80	0.26	63,63,63,63	0
58	MG	2w	104	1/1	0.80	0.14	67,67,67,67	0
58	MG	1a	1674	1/1	0.81	0.14	64,64,64,64	0
58	MG	2A	3127	1/1	0.81	0.20	30,30,30,30	0
58	MG	2a	1641	1/1	0.81	0.43	62,62,62,62	0
58	MG	1a	1678	1/1	0.81	0.38	49,49,49,49	0
58	MG	1A	3454	1/1	0.81	0.19	54,54,54,54	0
58	MG	2a	1659	1/1	0.81	0.12	77,77,77,77	0
58	MG	2A	3804	1/1	0.81	0.16	66,66,66,66	0
58	MG	1V	205	1/1	0.81	0.21	49,49,49,49	0
58	MG	2A	3320	1/1	0.81	0.34	57,57,57,57	0
58	MG	2A	3203	1/1	0.81	0.28	67,67,67,67	0
58	MG	1X	105	1/1	0.81	0.13	32,32,32,32	0
58	MG	2A	3341	1/1	0.81	0.11	66,66,66,66	0
58	MG	2a	1698	1/1	0.81	0.12	60,60,60,60	0
58	MG	1A	3783	1/1	0.81	0.12	46,46,46,46	0
58	MG	1Z	303	1/1	0.81	0.14	51,51,51,51	0
58	MG	2A	3619	1/1	0.81	0.21	50,50,50,50	0
58	MG	2A	3016	1/1	0.81	0.34	60,60,60,60	0
58	MG	2A	3241	1/1	0.81	0.22	54,54,54,54	0
58	MG	1A	3255	1/1	0.81	0.26	53,53,53,53	0
58	MG	14	101	1/1	0.81	0.11	58,58,58,58	0
58	MG	2A	3647	1/1	0.81	0.18	42,42,42,42	0
58	MG	1A	3944	1/1	0.81	0.09	52,52,52,52	0
58	MG	1A	3974	1/1	0.81	0.11	41,41,41,41	0
58	MG	2A	3684	1/1	0.81	0.45	73,73,73,73	0
58	MG	2a	1782	1/1	0.81	0.11	70,70,70,70	0
58	MG	1A	3693	1/1	0.81	0.18	56,56,56,56	0
58	MG	2A	3445	1/1	0.81	0.22	48,48,48,48	0
58	MG	2W	202	1/1	0.81	0.21	47,47,47,47	0
58	MG	2A	3447	1/1	0.81	0.20	52,52,52,52	0
58	MG	2A	3266	1/1	0.81	0.25	50,50,50,50	0
58	MG	2a	1604	1/1	0.81	0.16	65,65,65,65	0
58	MG	1A	3452	1/1	0.81	0.28	48,48,48,48	0
58	MG	1N	202	1/1	0.81	0.20	48,48,48,48	0
58	MG	2A	3717	1/1	0.81	0.32	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3278	1/1	0.81	0.26	58,58,58,58	0
58	MG	1A	3498	1/1	0.81	0.19	37,37,37,37	0
58	MG	2x	105	1/1	0.81	0.29	59,59,59,59	0
58	MG	2A	3225	1/1	0.82	0.16	57,57,57,57	0
58	MG	1A	3443	1/1	0.82	0.12	52,52,52,52	0
58	MG	2A	3412	1/1	0.82	0.25	39,39,39,39	0
58	MG	1a	1688	1/1	0.82	0.18	51,51,51,51	0
58	MG	2A	3438	1/1	0.82	0.12	64,64,64,64	0
58	MG	1a	1692	1/1	0.82	0.29	60,60,60,60	0
58	MG	2A	3723	1/1	0.82	0.18	43,43,43,43	0
58	MG	1A	3527	1/1	0.82	0.12	66,66,66,66	0
58	MG	1x	105	1/1	0.82	0.15	53,53,53,53	0
58	MG	1x	106	1/1	0.82	0.38	54,54,54,54	0
58	MG	2A	3768	1/1	0.82	0.26	37,37,37,37	0
58	MG	2A	3006	1/1	0.82	0.16	51,51,51,51	0
58	MG	1V	206	1/1	0.82	0.18	51,51,51,51	0
58	MG	2A	3018	1/1	0.82	0.19	48,48,48,48	0
58	MG	1A	4038	1/1	0.82	0.09	42,42,42,42	0
58	MG	2A	3510	1/1	0.82	0.21	59,59,59,59	0
58	MG	1A	3894	1/1	0.82	0.12	33,33,33,33	0
58	MG	1a	1740	1/1	0.82	0.18	56,56,56,56	0
58	MG	2A	3281	1/1	0.82	0.20	48,48,48,48	0
58	MG	1A	3678	1/1	0.82	0.12	34,34,34,34	0
58	MG	1a	1746	1/1	0.82	0.13	49,49,49,49	0
58	MG	2A	3554	1/1	0.82	0.08	49,49,49,49	0
58	MG	1B	225	1/1	0.82	0.15	57,57,57,57	0
58	MG	1A	3132	1/1	0.82	0.25	36,36,36,36	0
58	MG	2a	1761	1/1	0.82	0.09	63,63,63,63	0
58	MG	1a	1603	1/1	0.82	0.12	60,60,60,60	0
58	MG	2a	1772	1/1	0.82	0.16	61,61,61,61	0
58	MG	2A	3105	1/1	0.82	0.32	64,64,64,64	0
58	MG	1a	1607	1/1	0.82	0.35	57,57,57,57	0
58	MG	2A	3126	1/1	0.82	0.12	58,58,58,58	0
58	MG	2A	3330	1/1	0.82	0.27	68,68,68,68	0
58	MG	1A	4004	1/1	0.82	0.14	44,44,44,44	0
58	MG	2a	1809	1/1	0.82	0.19	61,61,61,61	0
58	MG	2E	301	1/1	0.82	0.22	51,51,51,51	0
58	MG	1A	3309	1/1	0.82	0.30	54,54,54,54	0
58	MG	1A	4027	1/1	0.82	0.17	61,61,61,61	0
58	MG	1G	203	1/1	0.82	0.13	50,50,50,50	0
58	MG	2A	3655	1/1	0.82	0.20	58,58,58,58	0
58	MG	1A	3612	1/1	0.82	0.28	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3672	1/1	0.82	0.30	51,51,51,51	0
58	MG	2A	3207	1/1	0.82	0.20	53,53,53,53	0
58	MG	1A	4069	1/1	0.82	0.11	30,30,30,30	0
58	MG	1O	203	1/1	0.82	0.19	58,58,58,58	0
58	MG	2A	3800	1/1	0.83	0.18	57,57,57,57	0
58	MG	1A	3546	1/1	0.83	0.24	48,48,48,48	0
58	MG	2a	1649	1/1	0.83	0.06	68,68,68,68	0
58	MG	1G	204	1/1	0.83	0.16	60,60,60,60	0
58	MG	2A	3135	1/1	0.83	0.18	38,38,38,38	0
58	MG	1A	4049	1/1	0.83	0.09	56,56,56,56	0
58	MG	2A	3325	1/1	0.83	0.20	46,46,46,46	0
58	MG	2A	3329	1/1	0.83	0.17	53,53,53,53	0
58	MG	2A	3825	1/1	0.83	0.15	55,55,55,55	0
58	MG	1A	3654	1/1	0.83	0.20	52,52,52,52	0
58	MG	2A	3333	1/1	0.83	0.21	48,48,48,48	0
58	MG	1A	4016	1/1	0.83	0.16	21,21,21,21	0
58	MG	2A	3193	1/1	0.83	0.29	46,46,46,46	0
58	MG	2a	1715	1/1	0.83	0.23	53,53,53,53	0
58	MG	2A	3200	1/1	0.83	0.21	50,50,50,50	0
58	MG	1a	1679	1/1	0.83	0.11	55,55,55,55	0
58	MG	1a	1681	1/1	0.83	0.19	61,61,61,61	0
58	MG	1A	3319	1/1	0.83	0.23	43,43,43,43	0
58	MG	1A	3160	1/1	0.83	0.18	49,49,49,49	0
58	MG	1A	3663	1/1	0.83	0.20	34,34,34,34	0
58	MG	1A	4081	1/1	0.83	0.20	40,40,40,40	0
58	MG	1A	4084	1/1	0.83	0.12	36,36,36,36	0
58	MG	1A	3881	1/1	0.83	0.21	38,38,38,38	0
58	MG	1A	3608	1/1	0.83	0.32	51,51,51,51	0
58	MG	1A	3506	1/1	0.83	0.18	32,32,32,32	0
58	MG	1B	230	1/1	0.83	0.08	54,54,54,54	0
58	MG	1A	3524	1/1	0.83	0.20	42,42,42,42	0
58	MG	2A	3046	1/1	0.83	0.18	48,48,48,48	0
58	MG	1a	1760	1/1	0.83	0.12	64,64,64,64	0
58	MG	2a	1607	1/1	0.83	0.12	64,64,64,64	0
58	MG	1A	3803	1/1	0.83	0.20	49,49,49,49	0
58	MG	1A	3372	1/1	0.83	0.23	38,38,38,38	0
58	MG	1a	1627	1/1	0.83	0.10	51,51,51,51	0
58	MG	2a	1626	1/1	0.83	0.22	55,55,55,55	0
58	MG	1a	1779	1/1	0.83	0.10	56,56,56,56	0
58	MG	1A	3701	1/1	0.83	0.18	20,20,20,20	0
58	MG	2A	3109	1/1	0.83	0.11	72,72,72,72	0
58	MG	1a	1642	1/1	0.83	0.23	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3112	1/1	0.83	0.10	47,47,47,47	0
58	MG	1a	1671	1/1	0.84	0.24	50,50,50,50	0
58	MG	2A	3761	1/1	0.84	0.18	63,63,63,63	0
58	MG	2A	3011	1/1	0.84	0.22	39,39,39,39	0
58	MG	2A	3774	1/1	0.84	0.13	44,44,44,44	0
58	MG	2a	1642	1/1	0.84	0.20	62,62,62,62	0
58	MG	1A	3954	1/1	0.84	0.15	29,29,29,29	0
58	MG	2A	3202	1/1	0.84	0.18	55,55,55,55	0
58	MG	2A	3323	1/1	0.84	0.22	57,57,57,57	0
58	MG	1A	3253	1/1	0.84	0.15	46,46,46,46	0
58	MG	1A	3185	1/1	0.84	0.14	44,44,44,44	0
58	MG	1A	3040	1/1	0.84	0.28	47,47,47,47	0
58	MG	2a	1664	1/1	0.84	0.18	58,58,58,58	0
58	MG	1A	3725	1/1	0.84	0.20	52,52,52,52	0
58	MG	2a	1667	1/1	0.84	0.12	55,55,55,55	0
58	MG	2a	1669	1/1	0.84	0.10	53,53,53,53	0
58	MG	1a	1682	1/1	0.84	0.22	58,58,58,58	0
58	MG	2A	3603	1/1	0.84	0.20	62,62,62,62	0
58	MG	1A	3814	1/1	0.84	0.19	40,40,40,40	0
58	MG	2a	1695	1/1	0.84	0.10	61,61,61,61	0
58	MG	2A	3063	1/1	0.84	0.41	64,64,64,64	0
58	MG	2A	3345	1/1	0.84	0.21	57,57,57,57	0
58	MG	2a	1713	1/1	0.84	0.29	51,51,51,51	0
58	MG	1A	4024	1/1	0.84	0.13	43,43,43,43	0
58	MG	2A	3349	1/1	0.84	0.14	60,60,60,60	0
58	MG	2a	1717	1/1	0.84	0.22	56,56,56,56	0
58	MG	1a	1622	1/1	0.84	0.22	63,63,63,63	0
58	MG	2a	1727	1/1	0.84	0.27	53,53,53,53	0
58	MG	1a	1706	1/1	0.84	0.20	49,49,49,49	0
58	MG	1a	1802	1/1	0.84	0.10	51,51,51,51	0
58	MG	2A	3100	1/1	0.84	0.21	68,68,68,68	0
58	MG	1T	203	1/1	0.84	0.12	42,42,42,42	0
58	MG	1a	1728	1/1	0.84	0.26	54,54,54,54	0
58	MG	2D	302	1/1	0.84	0.50	55,55,55,55	0
58	MG	1A	3220	1/1	0.84	0.29	49,49,49,49	0
58	MG	1A	3267	1/1	0.84	0.17	50,50,50,50	0
58	MG	1a	1737	1/1	0.84	0.16	57,57,57,57	0
58	MG	2F	303	1/1	0.84	0.28	51,51,51,51	0
58	MG	2F	304	1/1	0.84	0.15	47,47,47,47	0
58	MG	1a	1645	1/1	0.84	0.37	61,61,61,61	0
58	MG	1A	3173	1/1	0.84	0.18	51,51,51,51	0
58	MG	2A	3448	1/1	0.84	0.11	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3149	1/1	0.84	0.22	50,50,50,50	0
58	MG	2g	201	1/1	0.84	0.16	60,60,60,60	0
58	MG	2A	3468	1/1	0.84	0.21	58,58,58,58	0
58	MG	2a	1601	1/1	0.84	0.20	61,61,61,61	0
58	MG	2A	3294	1/1	0.84	0.35	54,54,54,54	0
58	MG	2A	3714	1/1	0.84	0.22	30,30,30,30	0
58	MG	1A	3695	1/1	0.84	0.18	31,31,31,31	0
58	MG	2A	3005	1/1	0.84	0.15	51,51,51,51	0
58	MG	2A	3492	1/1	0.84	0.23	46,46,46,46	0
58	MG	2A	3302	1/1	0.84	0.14	62,62,62,62	0
58	MG	2x	104	1/1	0.84	0.27	49,49,49,49	0
58	MG	2A	3755	1/1	0.84	0.11	40,40,40,40	0
58	MG	1A	3899	1/1	0.85	0.15	37,37,37,37	0
58	MG	1A	3920	1/1	0.85	0.15	33,33,33,33	0
58	MG	2A	3293	1/1	0.85	0.10	66,66,66,66	0
58	MG	1A	4042	1/1	0.85	0.07	39,39,39,39	0
58	MG	1A	3934	1/1	0.85	0.10	29,29,29,29	0
58	MG	2A	3297	1/1	0.85	0.24	38,38,38,38	0
58	MG	1a	1695	1/1	0.85	0.21	49,49,49,49	0
58	MG	1a	1697	1/1	0.85	0.14	56,56,56,56	0
58	MG	2A	3788	1/1	0.85	0.11	57,57,57,57	0
58	MG	1A	3831	1/1	0.85	0.14	34,34,34,34	0
58	MG	2A	3306	1/1	0.85	0.23	52,52,52,52	0
58	MG	2A	3311	1/1	0.85	0.21	35,35,35,35	0
58	MG	1A	3631	1/1	0.85	0.08	50,50,50,50	0
58	MG	2A	3540	1/1	0.85	0.19	58,58,58,58	0
58	MG	1A	3345	1/1	0.85	0.20	45,45,45,45	0
58	MG	2a	1681	1/1	0.85	0.11	57,57,57,57	0
58	MG	1w	105	1/1	0.85	0.37	59,59,59,59	0
58	MG	2A	3553	1/1	0.85	0.17	38,38,38,38	0
58	MG	2A	3188	1/1	0.85	0.16	46,46,46,46	0
58	MG	2A	3831	1/1	0.85	0.16	42,42,42,42	0
58	MG	2A	3563	1/1	0.85	0.33	38,38,38,38	0
58	MG	2A	3592	1/1	0.85	0.19	36,36,36,36	0
58	MG	1D	310	1/1	0.85	0.21	39,39,39,39	0
58	MG	1A	3475	1/1	0.85	0.29	59,59,59,59	0
58	MG	1F	313	1/1	0.85	0.17	34,34,34,34	0
58	MG	2a	1721	1/1	0.85	0.09	59,59,59,59	0
58	MG	2a	1722	1/1	0.85	0.25	71,71,71,71	0
58	MG	1A	4054	1/1	0.85	0.16	30,30,30,30	0
58	MG	1A	3417	1/1	0.85	0.20	45,45,45,45	0
58	MG	2a	1732	1/1	0.85	0.10	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3145	1/1	0.85	0.12	44,44,44,44	0
58	MG	1A	3747	1/1	0.85	0.13	54,54,54,54	0
58	MG	1a	1657	1/1	0.85	0.22	54,54,54,54	0
58	MG	1A	3804	1/1	0.85	0.20	43,43,43,43	0
58	MG	2A	3025	1/1	0.85	0.16	50,50,50,50	0
58	MG	1a	1763	1/1	0.85	0.14	58,58,58,58	0
58	MG	2A	3355	1/1	0.85	0.26	46,46,46,46	0
58	MG	1a	1766	1/1	0.85	0.21	49,49,49,49	0
58	MG	2A	3662	1/1	0.85	0.18	62,62,62,62	0
58	MG	2A	3366	1/1	0.85	0.11	50,50,50,50	0
58	MG	2A	3377	1/1	0.85	0.15	56,56,56,56	0
58	MG	2A	3045	1/1	0.85	0.18	61,61,61,61	0
58	MG	1A	3616	1/1	0.85	0.18	35,35,35,35	0
58	MG	1A	3781	1/1	0.85	0.17	25,25,25,25	0
58	MG	1A	3820	1/1	0.85	0.13	57,57,57,57	0
58	MG	1a	1675	1/1	0.85	0.22	62,62,62,62	0
58	MG	2a	1606	1/1	0.85	0.21	62,62,62,62	0
58	MG	1A	4101	1/1	0.85	0.12	46,46,46,46	0
58	MG	2l	202	1/1	0.85	0.11	62,62,62,62	0
58	MG	1a	1783	1/1	0.85	0.16	55,55,55,55	0
58	MG	2A	3439	1/1	0.85	0.20	45,45,45,45	0
58	MG	1A	4104	1/1	0.85	0.21	44,44,44,44	0
58	MG	2a	1621	1/1	0.85	0.14	51,51,51,51	0
58	MG	1a	1792	1/1	0.85	0.17	64,64,64,64	0
58	MG	2A	3101	1/1	0.85	0.27	61,61,61,61	0
58	MG	2A	3732	1/1	0.85	0.19	49,49,49,49	0
58	MG	2a	1632	1/1	0.85	0.17	55,55,55,55	0
60	ZN	2Y	202	1/1	0.85	0.06	86,86,86,86	0
58	MG	2A	3659	1/1	0.86	0.11	67,67,67,67	0
58	MG	1A	3911	1/1	0.86	0.26	45,45,45,45	0
58	MG	2A	3363	1/1	0.86	0.16	52,52,52,52	0
58	MG	2A	3670	1/1	0.86	0.12	51,51,51,51	0
58	MG	1a	1669	1/1	0.86	0.13	60,60,60,60	0
58	MG	2a	1616	1/1	0.86	0.24	64,64,64,64	0
58	MG	2A	3673	1/1	0.86	0.10	60,60,60,60	0
58	MG	1A	3347	1/1	0.86	0.14	39,39,39,39	0
58	MG	2A	3378	1/1	0.86	0.19	52,52,52,52	0
58	MG	2A	3685	1/1	0.86	0.20	49,49,49,49	0
58	MG	2A	3379	1/1	0.86	0.20	55,55,55,55	0
58	MG	1A	3360	1/1	0.86	0.23	43,43,43,43	0
58	MG	1A	4012	1/1	0.86	0.11	57,57,57,57	0
58	MG	2A	3402	1/1	0.86	0.10	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3295	1/1	0.86	0.20	40,40,40,40	0
58	MG	2A	3707	1/1	0.86	0.17	70,70,70,70	0
58	MG	1A	3720	1/1	0.86	0.17	40,40,40,40	0
58	MG	2A	3264	1/1	0.86	0.20	59,59,59,59	0
58	MG	2A	3419	1/1	0.86	0.35	36,36,36,36	0
58	MG	2A	3720	1/1	0.86	0.22	48,48,48,48	0
58	MG	2A	3420	1/1	0.86	0.37	48,48,48,48	0
58	MG	2A	3727	1/1	0.86	0.25	71,71,71,71	0
58	MG	1A	4094	1/1	0.86	0.21	38,38,38,38	0
58	MG	1A	3317	1/1	0.86	0.19	36,36,36,36	0
58	MG	1A	3382	1/1	0.86	0.23	41,41,41,41	0
58	MG	2A	3072	1/1	0.86	0.17	35,35,35,35	0
58	MG	1a	1793	1/1	0.86	0.11	54,54,54,54	0
58	MG	1A	3734	1/1	0.86	0.13	43,43,43,43	0
58	MG	2a	1690	1/1	0.86	0.19	51,51,51,51	0
58	MG	12	102	1/1	0.86	0.26	38,38,38,38	0
58	MG	2A	3457	1/1	0.86	0.21	45,45,45,45	0
58	MG	1a	1694	1/1	0.86	0.26	50,50,50,50	0
58	MG	2A	3108	1/1	0.86	0.19	47,47,47,47	0
58	MG	1a	1801	1/1	0.86	0.11	52,52,52,52	0
58	MG	1A	3559	1/1	0.86	0.23	42,42,42,42	0
58	MG	15	107	1/1	0.86	0.07	41,41,41,41	0
58	MG	2A	3114	1/1	0.86	0.23	55,55,55,55	0
58	MG	1A	3086	1/1	0.86	0.21	25,25,25,25	0
58	MG	1A	3189	1/1	0.86	0.27	40,40,40,40	0
58	MG	2a	1724	1/1	0.86	0.14	45,45,45,45	0
58	MG	2A	3812	1/1	0.86	0.18	34,34,34,34	0
58	MG	2A	3820	1/1	0.86	0.07	43,43,43,43	0
58	MG	1A	3571	1/1	0.86	0.25	27,27,27,27	0
58	MG	2a	1738	1/1	0.86	0.13	62,62,62,62	0
58	MG	2A	3517	1/1	0.86	0.19	59,59,59,59	0
58	MG	2A	3308	1/1	0.86	0.17	40,40,40,40	0
58	MG	2A	3136	1/1	0.86	0.18	41,41,41,41	0
58	MG	2A	3143	1/1	0.86	0.20	32,32,32,32	0
58	MG	1A	3606	1/1	0.86	0.11	56,56,56,56	0
58	MG	1w	103	1/1	0.86	0.17	46,46,46,46	0
58	MG	1a	1731	1/1	0.86	0.07	48,48,48,48	0
58	MG	1A	3485	1/1	0.86	0.23	37,37,37,37	0
58	MG	2A	3190	1/1	0.86	0.35	61,61,61,61	0
58	MG	1A	3889	1/1	0.86	0.23	35,35,35,35	0
58	MG	2a	1779	1/1	0.86	0.23	40,40,40,40	0
58	MG	1A	3988	1/1	0.86	0.12	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3334	1/1	0.86	0.24	57,57,57,57	0
58	MG	1x	107	1/1	0.86	0.31	53,53,53,53	0
58	MG	2a	1804	1/1	0.86	0.08	70,70,70,70	0
58	MG	1a	1638	1/1	0.86	0.15	45,45,45,45	0
58	MG	2a	1824	1/1	0.86	0.28	59,59,59,59	0
58	MG	2a	1829	1/1	0.86	0.11	46,46,46,46	0
58	MG	2D	306	1/1	0.86	0.32	48,48,48,48	0
58	MG	1a	1741	1/1	0.86	0.18	35,35,35,35	0
58	MG	1A	3006	1/1	0.86	0.23	50,50,50,50	0
58	MG	2k	201	1/1	0.86	0.29	55,55,55,55	0
58	MG	1A	3681	1/1	0.86	0.09	38,38,38,38	0
58	MG	2A	3218	1/1	0.86	0.13	58,58,58,58	0
58	MG	1A	3614	1/1	0.86	0.17	17,17,17,17	0
58	MG	2A	3352	1/1	0.86	0.33	54,54,54,54	0
58	MG	2v	102	1/1	0.86	0.20	46,46,46,46	0
58	MG	1A	4000	1/1	0.86	0.30	53,53,53,53	0
58	MG	2A	3357	1/1	0.86	0.21	58,58,58,58	0
58	MG	2A	3649	1/1	0.86	0.15	43,43,43,43	0
58	MG	25	106	1/1	0.86	0.25	57,57,57,57	0
58	MG	2A	3650	1/1	0.86	0.26	49,49,49,49	0
58	MG	2A	3360	1/1	0.86	0.26	57,57,57,57	0
58	MG	2A	3658	1/1	0.86	0.18	46,46,46,46	0
58	MG	1A	3302	1/1	0.87	0.23	30,30,30,30	0
58	MG	2a	1645	1/1	0.87	0.15	57,57,57,57	0
58	MG	2A	3760	1/1	0.87	0.17	57,57,57,57	0
58	MG	1A	3789	1/1	0.87	0.13	30,30,30,30	0
58	MG	2A	3524	1/1	0.87	0.09	61,61,61,61	0
58	MG	2a	1653	1/1	0.87	0.17	61,61,61,61	0
58	MG	1A	3306	1/1	0.87	0.41	34,34,34,34	0
58	MG	2A	3780	1/1	0.87	0.18	44,44,44,44	0
58	MG	1A	3246	1/1	0.87	0.12	38,38,38,38	0
58	MG	1A	3179	1/1	0.87	0.17	24,24,24,24	0
58	MG	1A	4001	1/1	0.87	0.15	50,50,50,50	0
58	MG	2A	3044	1/1	0.87	0.30	46,46,46,46	0
58	MG	1R	203	1/1	0.87	0.23	47,47,47,47	0
58	MG	2A	3221	1/1	0.87	0.26	40,40,40,40	0
58	MG	2A	3569	1/1	0.87	0.13	36,36,36,36	0
58	MG	2A	3586	1/1	0.87	0.25	27,27,27,27	0
58	MG	1A	3495	1/1	0.87	0.27	39,39,39,39	0
58	MG	1A	3399	1/1	0.87	0.30	52,52,52,52	0
58	MG	2A	3226	1/1	0.87	0.35	38,38,38,38	0
58	MG	2A	3054	1/1	0.87	0.18	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3265	1/1	0.87	0.20	50,50,50,50	0
58	MG	2A	3358	1/1	0.87	0.19	55,55,55,55	0
58	MG	2A	3238	1/1	0.87	0.08	64,64,64,64	0
58	MG	1W	202	1/1	0.87	0.24	45,45,45,45	0
58	MG	1X	102	1/1	0.87	0.16	37,37,37,37	0
58	MG	1A	3937	1/1	0.87	0.15	30,30,30,30	0
58	MG	2A	3638	1/1	0.87	0.30	43,43,43,43	0
58	MG	2A	3367	1/1	0.87	0.18	52,52,52,52	0
58	MG	2A	3851	1/1	0.87	0.38	53,53,53,53	0
58	MG	1A	3812	1/1	0.87	0.12	54,54,54,54	0
58	MG	1A	3626	1/1	0.87	0.22	23,23,23,23	0
58	MG	2A	3097	1/1	0.87	0.12	60,60,60,60	0
58	MG	2A	3380	1/1	0.87	0.13	47,47,47,47	0
58	MG	10	101	1/1	0.87	0.16	32,32,32,32	0
58	MG	1A	3249	1/1	0.87	0.16	44,44,44,44	0
58	MG	2A	3268	1/1	0.87	0.24	55,55,55,55	0
58	MG	1B	209	1/1	0.87	0.14	32,32,32,32	0
58	MG	1A	3508	1/1	0.87	0.26	44,44,44,44	0
58	MG	1a	1806	1/1	0.87	0.13	68,68,68,68	0
58	MG	1A	3272	1/1	0.87	0.22	45,45,45,45	0
58	MG	1a	1601	1/1	0.87	0.21	48,48,48,48	0
58	MG	1A	3292	1/1	0.87	0.18	42,42,42,42	0
58	MG	1a	1718	1/1	0.87	0.17	49,49,49,49	0
58	MG	1a	1604	1/1	0.87	0.17	54,54,54,54	0
58	MG	25	101	1/1	0.87	0.29	67,67,67,67	0
58	MG	2A	3131	1/1	0.87	0.15	42,42,42,42	0
58	MG	1A	3337	1/1	0.87	0.13	48,48,48,48	0
58	MG	2a	1806	1/1	0.87	0.14	47,47,47,47	0
58	MG	1A	3555	1/1	0.87	0.26	66,66,66,66	0
58	MG	2a	1817	1/1	0.87	0.31	65,65,65,65	0
58	MG	2A	3139	1/1	0.87	0.13	53,53,53,53	0
58	MG	2a	1828	1/1	0.87	0.26	58,58,58,58	0
58	MG	2a	1605	1/1	0.87	0.15	66,66,66,66	0
58	MG	2A	3452	1/1	0.87	0.29	41,41,41,41	0
58	MG	1A	3778	1/1	0.87	0.17	30,30,30,30	0
58	MG	1a	1619	1/1	0.87	0.10	48,48,48,48	0
58	MG	2A	3163	1/1	0.87	0.11	54,54,54,54	0
58	MG	2A	3166	1/1	0.87	0.32	53,53,53,53	0
58	MG	2A	3718	1/1	0.87	0.19	59,59,59,59	0
58	MG	1A	3190	1/1	0.87	0.14	47,47,47,47	0
58	MG	2a	1624	1/1	0.87	0.12	55,55,55,55	0
58	MG	2t	201	1/1	0.87	0.11	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3316	1/1	0.87	0.19	65,65,65,65	0
58	MG	1A	3876	1/1	0.87	0.25	45,45,45,45	0
58	MG	1A	3986	1/1	0.87	0.07	60,60,60,60	0
58	MG	2A	3735	1/1	0.87	0.13	65,65,65,65	0
58	MG	1A	3184	1/1	0.87	0.18	52,52,52,52	0
58	MG	2a	1637	1/1	0.87	0.14	57,57,57,57	0
58	MG	2A	3191	1/1	0.87	0.57	69,69,69,69	0
58	MG	2x	106	1/1	0.87	0.28	49,49,49,49	0
58	MG	2A	3515	1/1	0.87	0.25	33,33,33,33	0
58	MG	2A	3397	1/1	0.88	0.22	65,65,65,65	0
58	MG	1A	3830	1/1	0.88	0.11	50,50,50,50	0
58	MG	11	104	1/1	0.88	0.10	34,34,34,34	0
58	MG	1A	3489	1/1	0.88	0.15	41,41,41,41	0
58	MG	2A	3250	1/1	0.88	0.24	59,59,59,59	0
58	MG	1A	3494	1/1	0.88	0.23	56,56,56,56	0
58	MG	1A	3389	1/1	0.88	0.21	53,53,53,53	0
58	MG	1A	3323	1/1	0.88	0.22	31,31,31,31	0
58	MG	2A	3421	1/1	0.88	0.28	48,48,48,48	0
58	MG	1a	1602	1/1	0.88	0.20	56,56,56,56	0
58	MG	2A	3059	1/1	0.88	0.11	47,47,47,47	0
58	MG	1A	3858	1/1	0.88	0.14	44,44,44,44	0
58	MG	2A	3722	1/1	0.88	0.19	49,49,49,49	0
58	MG	2A	3440	1/1	0.88	0.31	53,53,53,53	0
58	MG	1A	3405	1/1	0.88	0.17	37,37,37,37	0
58	MG	2A	3066	1/1	0.88	0.33	50,50,50,50	0
58	MG	2a	1658	1/1	0.88	0.17	61,61,61,61	0
58	MG	1A	4109	1/1	0.88	0.35	50,50,50,50	0
58	MG	1B	208	1/1	0.88	0.13	48,48,48,48	0
58	MG	1A	3861	1/1	0.88	0.13	37,37,37,37	0
58	MG	2A	3754	1/1	0.88	0.15	63,63,63,63	0
58	MG	1A	3326	1/1	0.88	0.33	39,39,39,39	0
58	MG	1A	3334	1/1	0.88	0.23	37,37,37,37	0
58	MG	2A	3472	1/1	0.88	0.42	63,63,63,63	0
58	MG	1A	3744	1/1	0.88	0.20	70,70,70,70	0
58	MG	1A	3221	1/1	0.88	0.21	31,31,31,31	0
58	MG	2A	3773	1/1	0.88	0.20	46,46,46,46	0
58	MG	2A	3104	1/1	0.88	0.14	52,52,52,52	0
58	MG	1a	1780	1/1	0.88	0.07	62,62,62,62	0
58	MG	1A	3641	1/1	0.88	0.12	37,37,37,37	0
58	MG	1A	3774	1/1	0.88	0.13	26,26,26,26	0
58	MG	2a	1704	1/1	0.88	0.12	62,62,62,62	0
58	MG	1B	235	1/1	0.88	0.14	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3304	1/1	0.88	0.13	57,57,57,57	0
58	MG	2A	3512	1/1	0.88	0.09	65,65,65,65	0
58	MG	1A	3229	1/1	0.88	0.22	42,42,42,42	0
58	MG	1A	3651	1/1	0.88	0.13	53,53,53,53	0
58	MG	2A	3115	1/1	0.88	0.22	60,60,60,60	0
58	MG	2A	3810	1/1	0.88	0.18	45,45,45,45	0
58	MG	1E	309	1/1	0.88	0.18	21,21,21,21	0
58	MG	1A	4025	1/1	0.88	0.05	49,49,49,49	0
58	MG	2A	3535	1/1	0.88	0.14	28,28,28,28	0
58	MG	1A	3782	1/1	0.88	0.15	16,16,16,16	0
58	MG	2A	3317	1/1	0.88	0.38	50,50,50,50	0
58	MG	1A	3904	1/1	0.88	0.16	36,36,36,36	0
58	MG	2a	1741	1/1	0.88	0.13	52,52,52,52	0
58	MG	2A	3837	1/1	0.88	0.07	47,47,47,47	0
58	MG	1A	3529	1/1	0.88	0.14	47,47,47,47	0
58	MG	1A	3919	1/1	0.88	0.13	38,38,38,38	0
58	MG	2a	1754	1/1	0.88	0.19	60,60,60,60	0
58	MG	1A	3539	1/1	0.88	0.17	50,50,50,50	0
58	MG	2A	3146	1/1	0.88	0.18	55,55,55,55	0
58	MG	2a	1762	1/1	0.88	0.17	56,56,56,56	0
58	MG	2A	3147	1/1	0.88	0.24	32,32,32,32	0
58	MG	1a	1807	1/1	0.88	0.15	67,67,67,67	0
58	MG	1A	3168	1/1	0.88	0.14	24,24,24,24	0
58	MG	1A	3793	1/1	0.88	0.20	53,53,53,53	0
58	MG	2A	3338	1/1	0.88	0.14	43,43,43,43	0
58	MG	2A	3609	1/1	0.88	0.17	50,50,50,50	0
58	MG	2a	1791	1/1	0.88	0.22	63,63,63,63	0
58	MG	2B	203	1/1	0.88	0.21	60,60,60,60	0
58	MG	2B	206	1/1	0.88	0.15	60,60,60,60	0
58	MG	1a	1813	1/1	0.88	0.24	53,53,53,53	0
58	MG	2A	3178	1/1	0.88	0.20	44,44,44,44	0
58	MG	2A	3179	1/1	0.88	0.27	63,63,63,63	0
58	MG	1A	3943	1/1	0.88	0.10	54,54,54,54	0
58	MG	1A	3170	1/1	0.88	0.21	38,38,38,38	0
58	MG	1A	3665	1/1	0.88	0.29	38,38,38,38	0
58	MG	2A	3625	1/1	0.88	0.10	36,36,36,36	0
58	MG	2A	3635	1/1	0.88	0.11	54,54,54,54	0
58	MG	1A	3270	1/1	0.88	0.17	49,49,49,49	0
58	MG	1A	3674	1/1	0.88	0.15	45,45,45,45	0
58	MG	1A	3363	1/1	0.88	0.25	65,65,65,65	0
58	MG	1A	3025	1/1	0.88	0.17	34,34,34,34	0
58	MG	1a	1702	1/1	0.88	0.26	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1Y	201	1/1	0.88	0.21	41,41,41,41	0
58	MG	1A	3062	1/1	0.88	0.10	44,44,44,44	0
58	MG	1a	1711	1/1	0.88	0.19	50,50,50,50	0
58	MG	2a	1603	1/1	0.88	0.18	56,56,56,56	0
58	MG	1a	1712	1/1	0.88	0.14	46,46,46,46	0
58	MG	2w	101	1/1	0.88	0.21	44,44,44,44	0
58	MG	2A	3375	1/1	0.88	0.10	64,64,64,64	0
58	MG	1a	1713	1/1	0.88	0.31	57,57,57,57	0
58	MG	1A	3690	1/1	0.88	0.14	44,44,44,44	0
58	MG	1A	3080	1/1	0.88	0.18	55,55,55,55	0
58	MG	2A	3029	1/1	0.88	0.29	41,41,41,41	0
58	MG	2A	3033	1/1	0.88	0.25	32,32,32,32	0
58	MG	2A	3392	1/1	0.88	0.31	56,56,56,56	0
58	MG	2T	203	1/1	0.89	0.11	47,47,47,47	0
58	MG	2U	201	1/1	0.89	0.18	38,38,38,38	0
58	MG	2A	3332	1/1	0.89	0.20	50,50,50,50	0
58	MG	1a	1789	1/1	0.89	0.11	40,40,40,40	0
58	MG	20	103	1/1	0.89	0.13	46,46,46,46	0
58	MG	1A	3093	1/1	0.89	0.24	21,21,21,21	0
58	MG	1A	3978	1/1	0.89	0.26	49,49,49,49	0
58	MG	1A	3825	1/1	0.89	0.11	56,56,56,56	0
58	MG	1A	3293	1/1	0.89	0.28	27,27,27,27	0
58	MG	2A	3636	1/1	0.89	0.27	46,46,46,46	0
58	MG	1A	3537	1/1	0.89	0.19	31,31,31,31	0
58	MG	1a	1649	1/1	0.89	0.19	56,56,56,56	0
58	MG	2A	3155	1/1	0.89	0.12	45,45,45,45	0
58	MG	2A	3158	1/1	0.89	0.12	64,64,64,64	0
58	MG	1A	3438	1/1	0.89	0.19	30,30,30,30	0
58	MG	2A	3165	1/1	0.89	0.26	55,55,55,55	0
58	MG	2A	3654	1/1	0.89	0.24	43,43,43,43	0
58	MG	1A	3157	1/1	0.89	0.29	33,33,33,33	0
58	MG	2a	1618	1/1	0.89	0.09	60,60,60,60	0
58	MG	1A	3692	1/1	0.89	0.15	24,24,24,24	0
58	MG	1a	1667	1/1	0.89	0.11	58,58,58,58	0
58	MG	1A	3996	1/1	0.89	0.22	30,30,30,30	0
58	MG	2A	3665	1/1	0.89	0.10	59,59,59,59	0
58	MG	2A	3181	1/1	0.89	0.18	37,37,37,37	0
58	MG	2A	3184	1/1	0.89	0.16	35,35,35,35	0
58	MG	2a	1633	1/1	0.89	0.34	54,54,54,54	0
58	MG	1B	233	1/1	0.89	0.18	42,42,42,42	0
58	MG	2A	3187	1/1	0.89	0.40	59,59,59,59	0
58	MG	1A	3550	1/1	0.89	0.22	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3189	1/1	0.89	0.13	48,48,48,48	0
58	MG	1A	3024	1/1	0.89	0.18	50,50,50,50	0
58	MG	2a	1644	1/1	0.89	0.23	65,65,65,65	0
58	MG	1A	3096	1/1	0.89	0.16	31,31,31,31	0
58	MG	1A	3354	1/1	0.89	0.23	46,46,46,46	0
58	MG	2A	3693	1/1	0.89	0.24	61,61,61,61	0
58	MG	1A	4003	1/1	0.89	0.15	49,49,49,49	0
58	MG	2a	1652	1/1	0.89	0.13	49,49,49,49	0
58	MG	2A	3391	1/1	0.89	0.13	48,48,48,48	0
58	MG	2A	3705	1/1	0.89	0.17	51,51,51,51	0
58	MG	2A	3195	1/1	0.89	0.14	62,62,62,62	0
58	MG	1A	3074	1/1	0.89	0.34	57,57,57,57	0
58	MG	1G	202	1/1	0.89	0.20	45,45,45,45	0
58	MG	2A	3710	1/1	0.89	0.21	62,62,62,62	0
58	MG	1A	3458	1/1	0.89	0.19	41,41,41,41	0
58	MG	1A	3578	1/1	0.89	0.25	25,25,25,25	0
58	MG	2A	3407	1/1	0.89	0.24	54,54,54,54	0
58	MG	2a	1678	1/1	0.89	0.34	52,52,52,52	0
58	MG	2A	3213	1/1	0.89	0.12	56,56,56,56	0
58	MG	2A	3721	1/1	0.89	0.16	58,58,58,58	0
58	MG	1A	3882	1/1	0.89	0.26	37,37,37,37	0
58	MG	1x	109	1/1	0.89	0.10	50,50,50,50	0
58	MG	2A	3001	1/1	0.89	0.31	45,45,45,45	0
58	MG	1A	4021	1/1	0.89	0.11	30,30,30,30	0
58	MG	1A	3596	1/1	0.89	0.18	37,37,37,37	0
58	MG	2A	3428	1/1	0.89	0.26	33,33,33,33	0
58	MG	2A	3009	1/1	0.89	0.23	40,40,40,40	0
58	MG	2A	3752	1/1	0.89	0.19	42,42,42,42	0
58	MG	1A	3459	1/1	0.89	0.21	38,38,38,38	0
58	MG	1A	3205	1/1	0.89	0.13	43,43,43,43	0
58	MG	2A	3756	1/1	0.89	0.23	45,45,45,45	0
58	MG	1A	3609	1/1	0.89	0.20	58,58,58,58	0
58	MG	2A	3446	1/1	0.89	0.27	42,42,42,42	0
58	MG	1A	3758	1/1	0.89	0.10	55,55,55,55	0
58	MG	2A	3243	1/1	0.89	0.32	63,63,63,63	0
58	MG	1A	3465	1/1	0.89	0.17	56,56,56,56	0
58	MG	2a	1730	1/1	0.89	0.35	60,60,60,60	0
58	MG	1A	4037	1/1	0.89	0.21	50,50,50,50	0
58	MG	2a	1737	1/1	0.89	0.17	53,53,53,53	0
58	MG	1A	3473	1/1	0.89	0.24	53,53,53,53	0
58	MG	2A	3783	1/1	0.89	0.10	61,61,61,61	0
58	MG	2a	1740	1/1	0.89	0.38	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3211	1/1	0.89	0.17	60,60,60,60	0
58	MG	2A	3471	1/1	0.89	0.30	56,56,56,56	0
58	MG	1a	1724	1/1	0.89	0.28	53,53,53,53	0
58	MG	2a	1749	1/1	0.89	0.10	54,54,54,54	0
58	MG	1X	106	1/1	0.89	0.16	55,55,55,55	0
58	MG	2a	1753	1/1	0.89	0.15	56,56,56,56	0
58	MG	1A	3263	1/1	0.89	0.15	40,40,40,40	0
58	MG	2a	1757	1/1	0.89	0.12	66,66,66,66	0
58	MG	1A	3171	1/1	0.89	0.22	44,44,44,44	0
58	MG	2a	1760	1/1	0.89	0.10	62,62,62,62	0
58	MG	1A	3492	1/1	0.89	0.12	36,36,36,36	0
58	MG	1A	3941	1/1	0.89	0.10	41,41,41,41	0
58	MG	1A	3137	1/1	0.89	0.14	48,48,48,48	0
58	MG	2a	1768	1/1	0.89	0.10	57,57,57,57	0
58	MG	2A	3062	1/1	0.89	0.30	42,42,42,42	0
58	MG	1A	3226	1/1	0.89	0.35	53,53,53,53	0
58	MG	1A	3946	1/1	0.89	0.18	27,27,27,27	0
58	MG	2a	1777	1/1	0.89	0.20	53,53,53,53	0
58	MG	1a	1744	1/1	0.89	0.17	64,64,64,64	0
58	MG	1a	1745	1/1	0.89	0.08	59,59,59,59	0
58	MG	2a	1790	1/1	0.89	0.15	67,67,67,67	0
58	MG	1A	3948	1/1	0.89	0.19	58,58,58,58	0
58	MG	1a	1747	1/1	0.89	0.10	46,46,46,46	0
58	MG	1A	3400	1/1	0.89	0.18	29,29,29,29	0
58	MG	2a	1801	1/1	0.89	0.23	66,66,66,66	0
58	MG	2A	3084	1/1	0.89	0.29	48,48,48,48	0
58	MG	2A	3537	1/1	0.89	0.23	49,49,49,49	0
58	MG	2A	3085	1/1	0.89	0.35	38,38,38,38	0
58	MG	2a	1816	1/1	0.89	0.11	65,65,65,65	0
58	MG	18	104	1/1	0.89	0.29	43,43,43,43	0
58	MG	2A	3846	1/1	0.89	0.14	48,48,48,48	0
58	MG	1A	3500	1/1	0.89	0.27	48,48,48,48	0
58	MG	1a	1764	1/1	0.89	0.07	68,68,68,68	0
58	MG	1A	3325	1/1	0.89	0.18	46,46,46,46	0
58	MG	2a	1834	1/1	0.89	0.17	62,62,62,62	0
58	MG	2A	3860	1/1	0.89	0.24	42,42,42,42	0
58	MG	1a	1768	1/1	0.89	0.15	46,46,46,46	0
58	MG	1A	3502	1/1	0.89	0.22	39,39,39,39	0
58	MG	2A	3869	1/1	0.89	0.18	57,57,57,57	0
58	MG	2A	3580	1/1	0.89	0.14	50,50,50,50	0
58	MG	2A	3581	1/1	0.89	0.31	38,38,38,38	0
58	MG	1a	1772	1/1	0.89	0.09	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3088	1/1	0.89	0.24	24,24,24,24	0
58	MG	1A	3420	1/1	0.89	0.12	43,43,43,43	0
58	MG	1A	3960	1/1	0.89	0.11	58,58,58,58	0
58	MG	2A	3597	1/1	0.89	0.22	51,51,51,51	0
58	MG	2E	306	1/1	0.89	0.17	54,54,54,54	0
58	MG	1A	3520	1/1	0.89	0.18	29,29,29,29	0
58	MG	1A	3963	1/1	0.89	0.13	43,43,43,43	0
58	MG	2A	3611	1/1	0.89	0.13	57,57,57,57	0
58	MG	2P	201	1/1	0.89	0.16	46,46,46,46	0
58	MG	1A	3431	1/1	0.89	0.16	41,41,41,41	0
58	MG	1a	1784	1/1	0.89	0.11	40,40,40,40	0
60	ZN	2n	102	1/1	0.89	0.05	77,77,77,77	0
58	MG	1A	3788	1/1	0.90	0.15	34,34,34,34	0
58	MG	1a	1662	1/1	0.90	0.22	48,48,48,48	0
58	MG	1A	3472	1/1	0.90	0.19	49,49,49,49	0
58	MG	1A	3019	1/1	0.90	0.28	33,33,33,33	0
58	MG	1A	3795	1/1	0.90	0.08	49,49,49,49	0
58	MG	1A	3377	1/1	0.90	0.28	35,35,35,35	0
58	MG	2A	3652	1/1	0.90	0.18	59,59,59,59	0
58	MG	1A	3910	1/1	0.90	0.14	29,29,29,29	0
58	MG	1a	1810	1/1	0.90	0.11	46,46,46,46	0
58	MG	2A	3176	1/1	0.90	0.18	47,47,47,47	0
58	MG	1A	4009	1/1	0.90	0.20	18,18,18,18	0
58	MG	1A	3129	1/1	0.90	0.19	45,45,45,45	0
58	MG	2a	1619	1/1	0.90	0.42	56,56,56,56	0
58	MG	1A	3917	1/1	0.90	0.25	37,37,37,37	0
58	MG	1e	201	1/1	0.90	0.19	53,53,53,53	0
58	MG	1F	306	1/1	0.90	0.21	27,27,27,27	0
58	MG	2A	3369	1/1	0.90	0.20	51,51,51,51	0
58	MG	1A	3702	1/1	0.90	0.14	25,25,25,25	0
58	MG	2A	3675	1/1	0.90	0.19	51,51,51,51	0
58	MG	2A	3680	1/1	0.90	0.16	48,48,48,48	0
58	MG	2A	3682	1/1	0.90	0.17	46,46,46,46	0
58	MG	2a	1636	1/1	0.90	0.14	73,73,73,73	0
58	MG	1F	314	1/1	0.90	0.14	40,40,40,40	0
58	MG	1a	1686	1/1	0.90	0.11	49,49,49,49	0
58	MG	1A	4023	1/1	0.90	0.18	29,29,29,29	0
58	MG	1A	3707	1/1	0.90	0.12	34,34,34,34	0
58	MG	1A	3715	1/1	0.90	0.13	26,26,26,26	0
58	MG	2A	3387	1/1	0.90	0.14	55,55,55,55	0
58	MG	2A	3696	1/1	0.90	0.10	56,56,56,56	0
58	MG	1A	3935	1/1	0.90	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
58	MG	1A	3805	1/1	0.90	0.25	41,41,41,41	0
58	MG	2A	3199	1/1	0.90	0.21	37,37,37,37	0
58	MG	1A	3807	1/1	0.90	0.23	15,15,15,15	0
58	MG	1A	3510	1/1	0.90	0.16	39,39,39,39	0
58	MG	1A	4036	1/1	0.90	0.10	28,28,28,28	0
58	MG	2A	3205	1/1	0.90	0.13	56,56,56,56	0
58	MG	1A	3719	1/1	0.90	0.21	31,31,31,31	0
58	MG	2a	1662	1/1	0.90	0.51	68,68,68,68	0
58	MG	2A	3208	1/1	0.90	0.20	45,45,45,45	0
58	MG	2A	3212	1/1	0.90	0.21	57,57,57,57	0
58	MG	1A	3514	1/1	0.90	0.31	45,45,45,45	0
58	MG	2A	3215	1/1	0.90	0.26	53,53,53,53	0
58	MG	1A	3818	1/1	0.90	0.19	20,20,20,20	0
58	MG	2A	3022	1/1	0.90	0.20	35,35,35,35	0
58	MG	2A	3435	1/1	0.90	0.31	58,58,58,58	0
58	MG	1A	3950	1/1	0.90	0.13	43,43,43,43	0
58	MG	2a	1687	1/1	0.90	0.14	57,57,57,57	0
58	MG	2A	3733	1/1	0.90	0.18	55,55,55,55	0
58	MG	1a	1717	1/1	0.90	0.14	55,55,55,55	0
58	MG	1A	3487	1/1	0.90	0.23	30,30,30,30	0
58	MG	1A	3821	1/1	0.90	0.17	37,37,37,37	0
58	MG	2a	1703	1/1	0.90	0.17	52,52,52,52	0
58	MG	1A	4044	1/1	0.90	0.08	43,43,43,43	0
58	MG	1A	3953	1/1	0.90	0.11	23,23,23,23	0
58	MG	1A	3824	1/1	0.90	0.20	52,52,52,52	0
58	MG	2A	3239	1/1	0.90	0.32	46,46,46,46	0
58	MG	1a	1733	1/1	0.90	0.22	36,36,36,36	0
58	MG	1A	3724	1/1	0.90	0.10	55,55,55,55	0
58	MG	1A	3589	1/1	0.90	0.15	54,54,54,54	0
58	MG	1A	3329	1/1	0.90	0.29	60,60,60,60	0
58	MG	2A	3770	1/1	0.90	0.17	49,49,49,49	0
58	MG	2A	3057	1/1	0.90	0.12	65,65,65,65	0
58	MG	1A	3597	1/1	0.90	0.19	42,42,42,42	0
58	MG	11	106	1/1	0.90	0.13	43,43,43,43	0
58	MG	1A	4063	1/1	0.90	0.18	36,36,36,36	0
58	MG	2A	3785	1/1	0.90	0.12	40,40,40,40	0
58	MG	1A	3848	1/1	0.90	0.18	47,47,47,47	0
58	MG	2A	3494	1/1	0.90	0.25	40,40,40,40	0
58	MG	1A	3525	1/1	0.90	0.11	53,53,53,53	0
58	MG	1A	3748	1/1	0.90	0.17	37,37,37,37	0
58	MG	2a	1743	1/1	0.90	0.34	54,54,54,54	0
58	MG	18	105	1/1	0.90	0.24	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1a	1754	1/1	0.90	0.23	64,64,64,64	0
58	MG	1A	3366	1/1	0.90	0.17	48,48,48,48	0
58	MG	2a	1750	1/1	0.90	0.16	79,79,79,79	0
58	MG	2A	3075	1/1	0.90	0.21	35,35,35,35	0
58	MG	2A	3282	1/1	0.90	0.16	53,53,53,53	0
58	MG	2A	3077	1/1	0.90	0.19	49,49,49,49	0
58	MG	2A	3819	1/1	0.90	0.31	43,43,43,43	0
58	MG	2A	3079	1/1	0.90	0.22	42,42,42,42	0
58	MG	2A	3081	1/1	0.90	0.26	42,42,42,42	0
58	MG	2A	3530	1/1	0.90	0.06	53,53,53,53	0
58	MG	2A	3534	1/1	0.90	0.09	45,45,45,45	0
58	MG	1A	3751	1/1	0.90	0.10	45,45,45,45	0
58	MG	1A	3981	1/1	0.90	0.17	47,47,47,47	0
58	MG	2A	3087	1/1	0.90	0.28	41,41,41,41	0
58	MG	2A	3300	1/1	0.90	0.27	52,52,52,52	0
58	MG	2A	3088	1/1	0.90	0.12	65,65,65,65	0
58	MG	1A	4085	1/1	0.90	0.12	31,31,31,31	0
58	MG	2A	3303	1/1	0.90	0.20	56,56,56,56	0
58	MG	2A	3559	1/1	0.90	0.33	52,52,52,52	0
58	MG	2a	1786	1/1	0.90	0.22	43,43,43,43	0
58	MG	2a	1787	1/1	0.90	0.15	59,59,59,59	0
58	MG	1a	1605	1/1	0.90	0.15	41,41,41,41	0
58	MG	2A	3849	1/1	0.90	0.12	48,48,48,48	0
58	MG	2A	3565	1/1	0.90	0.24	25,25,25,25	0
58	MG	1A	3437	1/1	0.90	0.13	38,38,38,38	0
58	MG	2A	3572	1/1	0.90	0.19	37,37,37,37	0
58	MG	1A	3286	1/1	0.90	0.14	37,37,37,37	0
58	MG	1A	3462	1/1	0.90	0.25	43,43,43,43	0
58	MG	2a	1807	1/1	0.90	0.24	47,47,47,47	0
58	MG	2A	3583	1/1	0.90	0.16	42,42,42,42	0
58	MG	2a	1814	1/1	0.90	0.19	49,49,49,49	0
58	MG	2A	3106	1/1	0.90	0.15	37,37,37,37	0
58	MG	1A	3875	1/1	0.90	0.28	39,39,39,39	0
58	MG	2a	1820	1/1	0.90	0.33	56,56,56,56	0
58	MG	1B	202	1/1	0.90	0.20	39,39,39,39	0
58	MG	2B	211	1/1	0.90	0.12	50,50,50,50	0
58	MG	2A	3595	1/1	0.90	0.10	59,59,59,59	0
58	MG	1A	3373	1/1	0.90	0.23	26,26,26,26	0
58	MG	1A	3993	1/1	0.90	0.14	36,36,36,36	0
58	MG	2f	202	1/1	0.90	0.24	58,58,58,58	0
58	MG	2A	3599	1/1	0.90	0.17	32,32,32,32	0
58	MG	1a	1630	1/1	0.90	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
58	MG	1a	1633	1/1	0.90	0.31	45,45,45,45	0
58	MG	2A	3119	1/1	0.90	0.26	28,28,28,28	0
58	MG	1A	3621	1/1	0.90	0.14	24,24,24,24	0
58	MG	2G	201	1/1	0.90	0.12	61,61,61,61	0
58	MG	2n	101	1/1	0.90	0.10	60,60,60,60	0
58	MG	1A	3686	1/1	0.90	0.21	19,19,19,19	0
58	MG	2R	202	1/1	0.90	0.30	55,55,55,55	0
58	MG	2A	3331	1/1	0.90	0.22	46,46,46,46	0
58	MG	1A	3624	1/1	0.90	0.20	29,29,29,29	0
58	MG	1B	228	1/1	0.90	0.14	35,35,35,35	0
58	MG	1B	229	1/1	0.90	0.20	37,37,37,37	0
58	MG	2V	202	1/1	0.90	0.25	55,55,55,55	0
58	MG	1a	1796	1/1	0.90	0.09	51,51,51,51	0
58	MG	2X	101	1/1	0.90	0.26	47,47,47,47	0
58	MG	2A	3626	1/1	0.90	0.10	57,57,57,57	0
58	MG	2A	3631	1/1	0.90	0.14	49,49,49,49	0
58	MG	1a	1653	1/1	0.90	0.13	39,39,39,39	0
58	MG	1a	1799	1/1	0.90	0.19	59,59,59,59	0
58	MG	1A	4071	1/1	0.91	0.14	34,34,34,34	0
58	MG	1A	3806	1/1	0.91	0.17	23,23,23,23	0
58	MG	2A	3598	1/1	0.91	0.21	36,36,36,36	0
58	MG	1a	1615	1/1	0.91	0.14	46,46,46,46	0
58	MG	1A	3109	1/1	0.91	0.18	24,24,24,24	0
58	MG	2A	3605	1/1	0.91	0.20	30,30,30,30	0
58	MG	1A	3680	1/1	0.91	0.12	35,35,35,35	0
58	MG	1A	3291	1/1	0.91	0.10	44,44,44,44	0
58	MG	1A	3479	1/1	0.91	0.21	51,51,51,51	0
58	MG	1A	4091	1/1	0.91	0.30	46,46,46,46	0
58	MG	20	101	1/1	0.91	0.39	49,49,49,49	0
58	MG	2A	3614	1/1	0.91	0.16	61,61,61,61	0
58	MG	1A	3481	1/1	0.91	0.29	35,35,35,35	0
58	MG	2A	3132	1/1	0.91	0.16	59,59,59,59	0
58	MG	1a	1635	1/1	0.91	0.20	48,48,48,48	0
58	MG	27	103	1/1	0.91	0.16	43,43,43,43	0
58	MG	28	101	1/1	0.91	0.14	52,52,52,52	0
58	MG	1A	3412	1/1	0.91	0.23	43,43,43,43	0
58	MG	2A	3624	1/1	0.91	0.06	56,56,56,56	0
58	MG	1a	1641	1/1	0.91	0.18	49,49,49,49	0
58	MG	1A	4102	1/1	0.91	0.28	42,42,42,42	0
58	MG	2A	3628	1/1	0.91	0.16	38,38,38,38	0
58	MG	1A	3568	1/1	0.91	0.28	37,37,37,37	0
58	MG	1A	3198	1/1	0.91	0.33	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2a	1608	1/1	0.91	0.12	67,67,67,67	0
58	MG	1A	3969	1/1	0.91	0.18	32,32,32,32	0
58	MG	1a	1652	1/1	0.91	0.15	32,32,32,32	0
58	MG	1B	204	1/1	0.91	0.29	52,52,52,52	0
58	MG	1A	3094	1/1	0.91	0.21	31,31,31,31	0
58	MG	2a	1617	1/1	0.91	0.10	67,67,67,67	0
58	MG	1A	3582	1/1	0.91	0.20	26,26,26,26	0
58	MG	1A	3423	1/1	0.91	0.19	43,43,43,43	0
58	MG	2A	3354	1/1	0.91	0.24	59,59,59,59	0
58	MG	2A	3168	1/1	0.91	0.22	55,55,55,55	0
58	MG	2A	3356	1/1	0.91	0.35	54,54,54,54	0
58	MG	2A	3169	1/1	0.91	0.17	61,61,61,61	0
58	MG	1A	3836	1/1	0.91	0.17	30,30,30,30	0
58	MG	1A	3839	1/1	0.91	0.12	29,29,29,29	0
58	MG	1A	3842	1/1	0.91	0.22	50,50,50,50	0
58	MG	1A	3493	1/1	0.91	0.21	43,43,43,43	0
58	MG	1e	202	1/1	0.91	0.19	54,54,54,54	0
58	MG	1a	1673	1/1	0.91	0.24	54,54,54,54	0
58	MG	1A	3250	1/1	0.91	0.22	48,48,48,48	0
58	MG	2A	3370	1/1	0.91	0.24	63,63,63,63	0
58	MG	1A	3598	1/1	0.91	0.22	39,39,39,39	0
58	MG	2A	3678	1/1	0.91	0.09	56,56,56,56	0
58	MG	1A	3183	1/1	0.91	0.12	49,49,49,49	0
58	MG	1x	102	1/1	0.91	0.41	52,52,52,52	0
58	MG	1x	104	1/1	0.91	0.15	43,43,43,43	0
58	MG	1A	3254	1/1	0.91	0.18	35,35,35,35	0
58	MG	2A	3383	1/1	0.91	0.34	45,45,45,45	0
58	MG	2A	3384	1/1	0.91	0.21	46,46,46,46	0
58	MG	1A	3499	1/1	0.91	0.20	41,41,41,41	0
58	MG	1A	3216	1/1	0.91	0.23	41,41,41,41	0
58	MG	1A	3361	1/1	0.91	0.11	56,56,56,56	0
58	MG	1A	3870	1/1	0.91	0.12	41,41,41,41	0
58	MG	2A	3700	1/1	0.91	0.22	41,41,41,41	0
58	MG	2A	3394	1/1	0.91	0.07	58,58,58,58	0
58	MG	2A	3004	1/1	0.91	0.48	48,48,48,48	0
58	MG	2A	3399	1/1	0.91	0.15	57,57,57,57	0
58	MG	1A	3735	1/1	0.91	0.17	39,39,39,39	0
58	MG	1A	3092	1/1	0.91	0.12	47,47,47,47	0
58	MG	1A	3055	1/1	0.91	0.12	34,34,34,34	0
58	MG	2A	3712	1/1	0.91	0.10	55,55,55,55	0
58	MG	2A	3206	1/1	0.91	0.23	44,44,44,44	0
58	MG	2A	3408	1/1	0.91	0.18	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2a	1689	1/1	0.91	0.14	58,58,58,58	0
58	MG	1A	3310	1/1	0.91	0.25	33,33,33,33	0
58	MG	1a	1698	1/1	0.91	0.27	50,50,50,50	0
58	MG	2A	3415	1/1	0.91	0.19	58,58,58,58	0
58	MG	1A	4011	1/1	0.91	0.10	55,55,55,55	0
58	MG	1A	3224	1/1	0.91	0.20	43,43,43,43	0
58	MG	1A	4014	1/1	0.91	0.25	37,37,37,37	0
58	MG	2A	3731	1/1	0.91	0.14	32,32,32,32	0
58	MG	2a	1710	1/1	0.91	0.20	55,55,55,55	0
58	MG	1A	3750	1/1	0.91	0.15	53,53,53,53	0
58	MG	1A	4018	1/1	0.91	0.18	42,42,42,42	0
58	MG	2A	3433	1/1	0.91	0.28	53,53,53,53	0
58	MG	2A	3739	1/1	0.91	0.08	53,53,53,53	0
58	MG	1A	4020	1/1	0.91	0.10	38,38,38,38	0
58	MG	2A	3036	1/1	0.91	0.33	50,50,50,50	0
58	MG	2A	3749	1/1	0.91	0.15	53,53,53,53	0
58	MG	1A	3513	1/1	0.91	0.16	50,50,50,50	0
58	MG	1A	3139	1/1	0.91	0.13	32,32,32,32	0
58	MG	1A	3767	1/1	0.91	0.20	57,57,57,57	0
58	MG	1a	1722	1/1	0.91	0.15	59,59,59,59	0
58	MG	1A	3896	1/1	0.91	0.17	31,31,31,31	0
58	MG	2A	3759	1/1	0.91	0.10	56,56,56,56	0
58	MG	1a	1726	1/1	0.91	0.31	55,55,55,55	0
58	MG	2A	3053	1/1	0.91	0.22	47,47,47,47	0
58	MG	2A	3242	1/1	0.91	0.17	42,42,42,42	0
58	MG	2A	3769	1/1	0.91	0.28	38,38,38,38	0
58	MG	2A	3453	1/1	0.91	0.46	56,56,56,56	0
58	MG	1A	3639	1/1	0.91	0.08	56,56,56,56	0
58	MG	2A	3463	1/1	0.91	0.27	35,35,35,35	0
58	MG	2A	3779	1/1	0.91	0.10	45,45,45,45	0
58	MG	2A	3466	1/1	0.91	0.17	47,47,47,47	0
58	MG	2A	3247	1/1	0.91	0.27	44,44,44,44	0
58	MG	2A	3055	1/1	0.91	0.23	38,38,38,38	0
58	MG	2a	1756	1/1	0.91	0.10	57,57,57,57	0
58	MG	2A	3252	1/1	0.91	0.17	64,64,64,64	0
58	MG	2A	3056	1/1	0.91	0.13	60,60,60,60	0
58	MG	2A	3481	1/1	0.91	0.15	59,59,59,59	0
58	MG	2A	3255	1/1	0.91	0.12	57,57,57,57	0
58	MG	1A	3777	1/1	0.91	0.11	25,25,25,25	0
58	MG	2a	1765	1/1	0.91	0.09	48,48,48,48	0
58	MG	2a	1766	1/1	0.91	0.14	55,55,55,55	0
58	MG	2A	3260	1/1	0.91	0.21	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3100	1/1	0.91	0.11	55,55,55,55	0
58	MG	2a	1771	1/1	0.91	0.26	57,57,57,57	0
58	MG	2A	3807	1/1	0.91	0.10	40,40,40,40	0
58	MG	2A	3495	1/1	0.91	0.33	57,57,57,57	0
58	MG	1A	3238	1/1	0.91	0.11	57,57,57,57	0
58	MG	2A	3811	1/1	0.91	0.15	47,47,47,47	0
58	MG	1A	3460	1/1	0.91	0.16	44,44,44,44	0
58	MG	2a	1781	1/1	0.91	0.20	49,49,49,49	0
58	MG	1A	3526	1/1	0.91	0.21	39,39,39,39	0
58	MG	2a	1784	1/1	0.91	0.27	53,53,53,53	0
58	MG	1A	3386	1/1	0.91	0.22	52,52,52,52	0
58	MG	1A	3921	1/1	0.91	0.18	45,45,45,45	0
58	MG	2A	3513	1/1	0.91	0.09	47,47,47,47	0
58	MG	2A	3269	1/1	0.91	0.14	43,43,43,43	0
58	MG	2A	3271	1/1	0.91	0.22	64,64,64,64	0
58	MG	1A	3528	1/1	0.91	0.18	47,47,47,47	0
58	MG	1A	3241	1/1	0.91	0.14	29,29,29,29	0
58	MG	2A	3526	1/1	0.91	0.14	49,49,49,49	0
58	MG	10	106	1/1	0.91	0.19	57,57,57,57	0
58	MG	2A	3074	1/1	0.91	0.12	58,58,58,58	0
58	MG	1A	3936	1/1	0.91	0.20	51,51,51,51	0
58	MG	2a	1811	1/1	0.91	0.14	56,56,56,56	0
58	MG	2A	3283	1/1	0.91	0.15	40,40,40,40	0
58	MG	1A	3660	1/1	0.91	0.19	25,25,25,25	0
58	MG	1a	1748	1/1	0.91	0.13	44,44,44,44	0
58	MG	2A	3850	1/1	0.91	0.18	49,49,49,49	0
58	MG	1A	3938	1/1	0.91	0.09	34,34,34,34	0
58	MG	1A	3662	1/1	0.91	0.16	48,48,48,48	0
58	MG	2A	3544	1/1	0.91	0.26	53,53,53,53	0
58	MG	1A	3397	1/1	0.91	0.21	47,47,47,47	0
58	MG	2A	3866	1/1	0.91	0.27	40,40,40,40	0
58	MG	1A	3799	1/1	0.91	0.12	34,34,34,34	0
58	MG	1A	3469	1/1	0.91	0.09	45,45,45,45	0
58	MG	2B	202	1/1	0.91	0.12	37,37,37,37	0
58	MG	2A	3093	1/1	0.91	0.25	52,52,52,52	0
58	MG	1A	3542	1/1	0.91	0.36	54,54,54,54	0
58	MG	1A	4062	1/1	0.91	0.07	44,44,44,44	0
58	MG	2l	203	1/1	0.91	0.24	60,60,60,60	0
58	MG	2B	210	1/1	0.91	0.08	49,49,49,49	0
58	MG	1A	3544	1/1	0.91	0.34	44,44,44,44	0
58	MG	2B	212	1/1	0.91	0.24	61,61,61,61	0
58	MG	2B	213	1/1	0.91	0.22	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2B	215	1/1	0.91	0.19	59,59,59,59	0
58	MG	2B	216	1/1	0.91	0.19	46,46,46,46	0
58	MG	1A	4065	1/1	0.91	0.27	30,30,30,30	0
58	MG	2D	303	1/1	0.91	0.15	46,46,46,46	0
58	MG	1A	3675	1/1	0.91	0.10	33,33,33,33	0
58	MG	2A	3582	1/1	0.91	0.18	43,43,43,43	0
58	MG	2A	3307	1/1	0.91	0.26	49,49,49,49	0
58	MG	1A	3273	1/1	0.91	0.21	28,28,28,28	0
58	MG	2A	3309	1/1	0.91	0.17	53,53,53,53	0
58	MG	1a	1775	1/1	0.91	0.09	68,68,68,68	0
58	MG	2A	3314	1/1	0.91	0.22	37,37,37,37	0
58	MG	1a	1612	1/1	0.92	0.13	51,51,51,51	0
58	MG	2A	3117	1/1	0.92	0.26	49,49,49,49	0
58	MG	2A	3607	1/1	0.92	0.26	56,56,56,56	0
58	MG	1A	3439	1/1	0.92	0.14	31,31,31,31	0
58	MG	2A	3610	1/1	0.92	0.19	56,56,56,56	0
58	MG	2A	3124	1/1	0.92	0.29	44,44,44,44	0
58	MG	1A	4096	1/1	0.92	0.20	71,71,71,71	0
58	MG	1A	3113	1/1	0.92	0.23	28,28,28,28	0
58	MG	1a	1621	1/1	0.92	0.23	46,46,46,46	0
58	MG	1a	1786	1/1	0.92	0.20	50,50,50,50	0
58	MG	2A	3133	1/1	0.92	0.17	46,46,46,46	0
58	MG	2A	3340	1/1	0.92	0.35	45,45,45,45	0
58	MG	1A	3666	1/1	0.92	0.19	34,34,34,34	0
58	MG	1A	3570	1/1	0.92	0.35	55,55,55,55	0
58	MG	21	101	1/1	0.92	0.14	44,44,44,44	0
58	MG	1A	4106	1/1	0.92	0.21	40,40,40,40	0
58	MG	1A	4107	1/1	0.92	0.37	51,51,51,51	0
58	MG	27	102	1/1	0.92	0.19	48,48,48,48	0
58	MG	1a	1794	1/1	0.92	0.10	39,39,39,39	0
58	MG	1A	4108	1/1	0.92	0.40	55,55,55,55	0
58	MG	2A	3351	1/1	0.92	0.11	68,68,68,68	0
58	MG	1A	3885	1/1	0.92	0.15	24,24,24,24	0
58	MG	2A	3353	1/1	0.92	0.16	44,44,44,44	0
58	MG	2A	3640	1/1	0.92	0.16	30,30,30,30	0
58	MG	1A	3149	1/1	0.92	0.26	25,25,25,25	0
58	MG	1A	3575	1/1	0.92	0.23	37,37,37,37	0
58	MG	2A	3159	1/1	0.92	0.22	42,42,42,42	0
58	MG	2A	3162	1/1	0.92	0.16	59,59,59,59	0
58	MG	1A	3117	1/1	0.92	0.15	35,35,35,35	0
58	MG	1a	1643	1/1	0.92	0.09	55,55,55,55	0
58	MG	1A	3790	1/1	0.92	0.13	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	4005	1/1	0.92	0.14	42,42,42,42	0
58	MG	1A	3153	1/1	0.92	0.15	27,27,27,27	0
58	MG	1B	219	1/1	0.92	0.17	38,38,38,38	0
58	MG	1a	1808	1/1	0.92	0.12	58,58,58,58	0
58	MG	1A	3584	1/1	0.92	0.17	31,31,31,31	0
58	MG	2A	3374	1/1	0.92	0.21	58,58,58,58	0
58	MG	1a	1656	1/1	0.92	0.19	47,47,47,47	0
58	MG	1A	3505	1/1	0.92	0.18	39,39,39,39	0
58	MG	2A	3182	1/1	0.92	0.44	51,51,51,51	0
58	MG	2A	3183	1/1	0.92	0.28	41,41,41,41	0
58	MG	2A	3677	1/1	0.92	0.37	48,48,48,48	0
58	MG	1a	1660	1/1	0.92	0.25	44,44,44,44	0
58	MG	1A	3592	1/1	0.92	0.26	55,55,55,55	0
58	MG	2A	3681	1/1	0.92	0.13	32,32,32,32	0
58	MG	2A	3186	1/1	0.92	0.26	44,44,44,44	0
58	MG	1a	1664	1/1	0.92	0.30	47,47,47,47	0
58	MG	1A	3914	1/1	0.92	0.25	41,41,41,41	0
58	MG	2A	3389	1/1	0.92	0.27	55,55,55,55	0
58	MG	1l	202	1/1	0.92	0.30	64,64,64,64	0
58	MG	1A	3378	1/1	0.92	0.30	39,39,39,39	0
58	MG	1A	3507	1/1	0.92	0.14	40,40,40,40	0
58	MG	1a	1670	1/1	0.92	0.27	45,45,45,45	0
58	MG	2a	1650	1/1	0.92	0.22	55,55,55,55	0
58	MG	1A	4019	1/1	0.92	0.18	20,20,20,20	0
58	MG	1A	3327	1/1	0.92	0.29	31,31,31,31	0
58	MG	1x	103	1/1	0.92	0.28	54,54,54,54	0
58	MG	1B	236	1/1	0.92	0.12	53,53,53,53	0
58	MG	1A	3126	1/1	0.92	0.20	22,22,22,22	0
58	MG	1D	305	1/1	0.92	0.17	22,22,22,22	0
58	MG	1A	3697	1/1	0.92	0.28	62,62,62,62	0
58	MG	1x	108	1/1	0.92	0.14	20,20,20,20	0
58	MG	1A	3698	1/1	0.92	0.15	26,26,26,26	0
58	MG	2A	3713	1/1	0.92	0.23	53,53,53,53	0
58	MG	1A	3700	1/1	0.92	0.15	33,33,33,33	0
58	MG	2a	1674	1/1	0.92	0.09	59,59,59,59	0
58	MG	2a	1675	1/1	0.92	0.26	40,40,40,40	0
58	MG	2A	3715	1/1	0.92	0.23	32,32,32,32	0
58	MG	1E	312	1/1	0.92	0.15	35,35,35,35	0
58	MG	1A	4026	1/1	0.92	0.17	57,57,57,57	0
58	MG	2A	3214	1/1	0.92	0.12	46,46,46,46	0
58	MG	2a	1684	1/1	0.92	0.14	54,54,54,54	0
58	MG	2A	3424	1/1	0.92	0.16	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1F	311	1/1	0.92	0.18	44,44,44,44	0
58	MG	2A	3429	1/1	0.92	0.18	30,30,30,30	0
58	MG	1A	3026	1/1	0.92	0.14	50,50,50,50	0
58	MG	1a	1693	1/1	0.92	0.37	52,52,52,52	0
58	MG	2A	3012	1/1	0.92	0.18	39,39,39,39	0
58	MG	2A	3015	1/1	0.92	0.17	42,42,42,42	0
58	MG	2A	3224	1/1	0.92	0.14	52,52,52,52	0
58	MG	1A	4029	1/1	0.92	0.12	35,35,35,35	0
58	MG	2A	3740	1/1	0.92	0.12	45,45,45,45	0
58	MG	2a	1712	1/1	0.92	0.20	58,58,58,58	0
58	MG	2A	3741	1/1	0.92	0.11	47,47,47,47	0
58	MG	2A	3742	1/1	0.92	0.26	46,46,46,46	0
58	MG	1A	3394	1/1	0.92	0.08	36,36,36,36	0
58	MG	1A	3705	1/1	0.92	0.22	25,25,25,25	0
58	MG	2a	1720	1/1	0.92	0.11	64,64,64,64	0
58	MG	2A	3747	1/1	0.92	0.20	60,60,60,60	0
58	MG	1A	4033	1/1	0.92	0.16	54,54,54,54	0
58	MG	1G	205	1/1	0.92	0.26	57,57,57,57	0
58	MG	1N	201	1/1	0.92	0.45	51,51,51,51	0
58	MG	2a	1726	1/1	0.92	0.17	46,46,46,46	0
58	MG	2A	3032	1/1	0.92	0.26	37,37,37,37	0
58	MG	2a	1728	1/1	0.92	0.13	49,49,49,49	0
58	MG	1A	3516	1/1	0.92	0.14	42,42,42,42	0
58	MG	2A	3458	1/1	0.92	0.26	51,51,51,51	0
58	MG	2A	3035	1/1	0.92	0.24	31,31,31,31	0
58	MG	1A	3166	1/1	0.92	0.26	53,53,53,53	0
58	MG	2A	3037	1/1	0.92	0.30	47,47,47,47	0
58	MG	1A	3615	1/1	0.92	0.13	23,23,23,23	0
58	MG	1A	3947	1/1	0.92	0.18	35,35,35,35	0
58	MG	1Q	205	1/1	0.92	0.14	61,61,61,61	0
58	MG	2a	1744	1/1	0.92	0.22	69,69,69,69	0
58	MG	2A	3771	1/1	0.92	0.22	50,50,50,50	0
58	MG	2A	3256	1/1	0.92	0.10	67,67,67,67	0
58	MG	1A	4039	1/1	0.92	0.19	19,19,19,19	0
58	MG	1A	3237	1/1	0.92	0.29	32,32,32,32	0
58	MG	2A	3491	1/1	0.92	0.23	43,43,43,43	0
58	MG	1A	3340	1/1	0.92	0.23	36,36,36,36	0
58	MG	2A	3784	1/1	0.92	0.29	48,48,48,48	0
58	MG	1A	3027	1/1	0.92	0.15	56,56,56,56	0
58	MG	1A	3266	1/1	0.92	0.27	34,34,34,34	0
58	MG	2A	3787	1/1	0.92	0.15	58,58,58,58	0
58	MG	2A	3497	1/1	0.92	0.23	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3798	1/1	0.92	0.14	46,46,46,46	0
58	MG	1A	3191	1/1	0.92	0.28	32,32,32,32	0
58	MG	1a	1729	1/1	0.92	0.16	47,47,47,47	0
58	MG	2A	3505	1/1	0.92	0.26	38,38,38,38	0
58	MG	2A	3506	1/1	0.92	0.15	51,51,51,51	0
58	MG	2A	3507	1/1	0.92	0.17	46,46,46,46	0
58	MG	2A	3806	1/1	0.92	0.18	47,47,47,47	0
58	MG	2A	3508	1/1	0.92	0.17	55,55,55,55	0
58	MG	1a	1730	1/1	0.92	0.10	58,58,58,58	0
58	MG	1A	3005	1/1	0.92	0.20	30,30,30,30	0
58	MG	1A	3311	1/1	0.92	0.22	47,47,47,47	0
58	MG	1A	3424	1/1	0.92	0.08	44,44,44,44	0
58	MG	1A	3362	1/1	0.92	0.18	33,33,33,33	0
58	MG	1A	4050	1/1	0.92	0.14	27,27,27,27	0
58	MG	2A	3519	1/1	0.92	0.18	33,33,33,33	0
58	MG	2A	3280	1/1	0.92	0.19	46,46,46,46	0
58	MG	2A	3523	1/1	0.92	0.15	36,36,36,36	0
58	MG	1a	1738	1/1	0.92	0.24	48,48,48,48	0
58	MG	1a	1739	1/1	0.92	0.19	57,57,57,57	0
58	MG	1A	3432	1/1	0.92	0.18	43,43,43,43	0
58	MG	2A	3285	1/1	0.92	0.25	47,47,47,47	0
58	MG	2A	3841	1/1	0.92	0.23	63,63,63,63	0
58	MG	2A	3288	1/1	0.92	0.27	67,67,67,67	0
58	MG	1A	3271	1/1	0.92	0.44	47,47,47,47	0
58	MG	2A	3536	1/1	0.92	0.13	45,45,45,45	0
58	MG	1a	1742	1/1	0.92	0.12	40,40,40,40	0
58	MG	1A	3853	1/1	0.92	0.18	51,51,51,51	0
58	MG	11	101	1/1	0.92	0.32	34,34,34,34	0
58	MG	1A	3652	1/1	0.92	0.15	14,14,14,14	0
58	MG	1A	3364	1/1	0.92	0.20	45,45,45,45	0
58	MG	2A	3551	1/1	0.92	0.16	37,37,37,37	0
58	MG	12	101	1/1	0.92	0.29	40,40,40,40	0
58	MG	2A	3861	1/1	0.92	0.21	50,50,50,50	0
58	MG	1A	3020	1/1	0.92	0.16	37,37,37,37	0
58	MG	13	104	1/1	0.92	0.15	51,51,51,51	0
58	MG	2A	3562	1/1	0.92	0.15	45,45,45,45	0
58	MG	1A	3368	1/1	0.92	0.18	45,45,45,45	0
58	MG	1A	3866	1/1	0.92	0.11	47,47,47,47	0
58	MG	2A	3566	1/1	0.92	0.26	47,47,47,47	0
58	MG	1a	1761	1/1	0.92	0.13	50,50,50,50	0
58	MG	2A	3098	1/1	0.92	0.24	39,39,39,39	0
58	MG	1A	3869	1/1	0.92	0.14	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3563	1/1	0.92	0.19	34,34,34,34	0
58	MG	1A	3872	1/1	0.92	0.08	54,54,54,54	0
58	MG	2A	3310	1/1	0.92	0.20	55,55,55,55	0
58	MG	2B	214	1/1	0.92	0.15	48,48,48,48	0
58	MG	2A	3584	1/1	0.92	0.11	59,59,59,59	0
58	MG	1A	4083	1/1	0.92	0.25	43,43,43,43	0
58	MG	1A	3775	1/1	0.92	0.16	23,23,23,23	0
58	MG	1A	3989	1/1	0.92	0.14	51,51,51,51	0
58	MG	2D	305	1/1	0.92	0.17	45,45,45,45	0
58	MG	1A	3497	1/1	0.92	0.14	45,45,45,45	0
58	MG	1A	4092	1/1	0.92	0.20	38,38,38,38	0
58	MG	1A	4093	1/1	0.92	0.15	42,42,42,42	0
58	MG	2E	303	1/1	0.92	0.19	59,59,59,59	0
58	MG	2A	3113	1/1	0.92	0.23	50,50,50,50	0
58	MG	1a	1778	1/1	0.92	0.10	46,46,46,46	0
60	ZN	24	501	1/1	0.92	0.06	99,99,99,99	0
58	MG	2A	3600	1/1	0.92	0.17	43,43,43,43	0
58	MG	2A	3228	1/1	0.93	0.23	47,47,47,47	0
58	MG	1A	3773	1/1	0.93	0.20	19,19,19,19	0
58	MG	2A	3418	1/1	0.93	0.35	39,39,39,39	0
58	MG	28	102	1/1	0.93	0.16	51,51,51,51	0
58	MG	2A	3235	1/1	0.93	0.25	49,49,49,49	0
58	MG	2A	3236	1/1	0.93	0.29	39,39,39,39	0
58	MG	15	106	1/1	0.93	0.15	27,27,27,27	0
58	MG	1A	3289	1/1	0.93	0.12	33,33,33,33	0
58	MG	17	103	1/1	0.93	0.18	31,31,31,31	0
58	MG	2A	3240	1/1	0.93	0.27	40,40,40,40	0
58	MG	18	102	1/1	0.93	0.15	40,40,40,40	0
58	MG	1A	4097	1/1	0.93	0.11	39,39,39,39	0
58	MG	2A	3691	1/1	0.93	0.10	63,63,63,63	0
58	MG	2A	3434	1/1	0.93	0.28	50,50,50,50	0
58	MG	2A	3694	1/1	0.93	0.10	47,47,47,47	0
58	MG	1A	4099	1/1	0.93	0.11	39,39,39,39	0
58	MG	1A	3877	1/1	0.93	0.20	55,55,55,55	0
58	MG	2A	3064	1/1	0.93	0.10	60,60,60,60	0
58	MG	2A	3703	1/1	0.93	0.26	53,53,53,53	0
58	MG	1A	3474	1/1	0.93	0.20	41,41,41,41	0
58	MG	2A	3441	1/1	0.93	0.53	52,52,52,52	0
58	MG	1A	3580	1/1	0.93	0.15	27,27,27,27	0
58	MG	1A	3393	1/1	0.93	0.22	29,29,29,29	0
58	MG	1A	3210	1/1	0.93	0.16	44,44,44,44	0
58	MG	1A	3480	1/1	0.93	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
58	MG	1A	3890	1/1	0.93	0.21	24,24,24,24	0
58	MG	1B	201	1/1	0.93	0.20	45,45,45,45	0
58	MG	1A	3395	1/1	0.93	0.26	28,28,28,28	0
58	MG	2A	3076	1/1	0.93	0.24	32,32,32,32	0
58	MG	2A	3716	1/1	0.93	0.19	39,39,39,39	0
58	MG	1a	1614	1/1	0.93	0.11	52,52,52,52	0
58	MG	1A	3784	1/1	0.93	0.19	34,34,34,34	0
58	MG	2a	1643	1/1	0.93	0.14	73,73,73,73	0
58	MG	1a	1767	1/1	0.93	0.24	41,41,41,41	0
58	MG	1A	3077	1/1	0.93	0.12	42,42,42,42	0
58	MG	1A	3898	1/1	0.93	0.20	38,38,38,38	0
58	MG	2A	3272	1/1	0.93	0.12	60,60,60,60	0
58	MG	2A	3725	1/1	0.93	0.18	35,35,35,35	0
58	MG	2A	3477	1/1	0.93	0.24	34,34,34,34	0
58	MG	1B	210	1/1	0.93	0.13	53,53,53,53	0
58	MG	1a	1623	1/1	0.93	0.19	54,54,54,54	0
58	MG	1a	1624	1/1	0.93	0.23	56,56,56,56	0
58	MG	1a	1626	1/1	0.93	0.09	53,53,53,53	0
58	MG	1A	3486	1/1	0.93	0.20	27,27,27,27	0
58	MG	1A	3442	1/1	0.93	0.21	45,45,45,45	0
58	MG	1A	3599	1/1	0.93	0.31	31,31,31,31	0
58	MG	2A	3102	1/1	0.93	0.23	40,40,40,40	0
58	MG	2A	3743	1/1	0.93	0.11	55,55,55,55	0
58	MG	2A	3496	1/1	0.93	0.20	42,42,42,42	0
58	MG	1A	3682	1/1	0.93	0.20	37,37,37,37	0
58	MG	2a	1673	1/1	0.93	0.20	55,55,55,55	0
58	MG	1A	3601	1/1	0.93	0.11	47,47,47,47	0
58	MG	1a	1637	1/1	0.93	0.14	43,43,43,43	0
58	MG	2A	3502	1/1	0.93	0.14	33,33,33,33	0
58	MG	1A	3915	1/1	0.93	0.15	44,44,44,44	0
58	MG	1A	3167	1/1	0.93	0.21	36,36,36,36	0
58	MG	1A	3918	1/1	0.93	0.17	42,42,42,42	0
58	MG	1A	3691	1/1	0.93	0.20	54,54,54,54	0
58	MG	2a	1685	1/1	0.93	0.14	56,56,56,56	0
58	MG	2A	3299	1/1	0.93	0.25	38,38,38,38	0
58	MG	2a	1688	1/1	0.93	0.07	62,62,62,62	0
58	MG	1A	3491	1/1	0.93	0.18	30,30,30,30	0
58	MG	1a	1646	1/1	0.93	0.14	33,33,33,33	0
58	MG	2A	3764	1/1	0.93	0.12	43,43,43,43	0
58	MG	2a	1692	1/1	0.93	0.24	55,55,55,55	0
58	MG	1a	1647	1/1	0.93	0.13	47,47,47,47	0
58	MG	1A	3532	1/1	0.93	0.23	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3118	1/1	0.93	0.16	45,45,45,45	0
58	MG	1A	3927	1/1	0.93	0.20	24,24,24,24	0
58	MG	1A	3933	1/1	0.93	0.11	29,29,29,29	0
58	MG	1A	3448	1/1	0.93	0.19	35,35,35,35	0
58	MG	2a	1711	1/1	0.93	0.16	59,59,59,59	0
58	MG	1A	3336	1/1	0.93	0.21	35,35,35,35	0
58	MG	1A	3217	1/1	0.93	0.15	48,48,48,48	0
58	MG	2A	3782	1/1	0.93	0.22	38,38,38,38	0
58	MG	1a	1658	1/1	0.93	0.15	49,49,49,49	0
58	MG	1A	3455	1/1	0.93	0.21	38,38,38,38	0
58	MG	2A	3533	1/1	0.93	0.16	36,36,36,36	0
58	MG	1A	3620	1/1	0.93	0.08	52,52,52,52	0
58	MG	1F	305	1/1	0.93	0.14	34,34,34,34	0
58	MG	2a	1723	1/1	0.93	0.24	61,61,61,61	0
58	MG	1A	3371	1/1	0.93	0.20	37,37,37,37	0
58	MG	1A	3297	1/1	0.93	0.13	47,47,47,47	0
58	MG	2A	3319	1/1	0.93	0.33	49,49,49,49	0
58	MG	2A	3145	1/1	0.93	0.17	43,43,43,43	0
58	MG	1F	312	1/1	0.93	0.17	44,44,44,44	0
58	MG	1a	1812	1/1	0.93	0.14	58,58,58,58	0
58	MG	2A	3549	1/1	0.93	0.13	41,41,41,41	0
58	MG	2a	1735	1/1	0.93	0.26	47,47,47,47	0
58	MG	1A	3551	1/1	0.93	0.19	46,46,46,46	0
58	MG	2A	3154	1/1	0.93	0.19	54,54,54,54	0
58	MG	1A	3945	1/1	0.93	0.16	31,31,31,31	0
58	MG	1A	3629	1/1	0.93	0.11	28,28,28,28	0
58	MG	1A	3553	1/1	0.93	0.14	41,41,41,41	0
58	MG	1A	3418	1/1	0.93	0.21	36,36,36,36	0
58	MG	2A	3815	1/1	0.93	0.23	31,31,31,31	0
58	MG	1m	3001	1/1	0.93	0.09	54,54,54,54	0
58	MG	2A	3164	1/1	0.93	0.19	33,33,33,33	0
58	MG	1A	3557	1/1	0.93	0.15	33,33,33,33	0
58	MG	2A	3570	1/1	0.93	0.22	51,51,51,51	0
58	MG	1A	3344	1/1	0.93	0.31	51,51,51,51	0
58	MG	2A	3577	1/1	0.93	0.17	43,43,43,43	0
58	MG	2A	3832	1/1	0.93	0.23	48,48,48,48	0
58	MG	1A	3011	1/1	0.93	0.15	37,37,37,37	0
58	MG	1w	107	1/1	0.93	0.11	57,57,57,57	0
58	MG	2A	3344	1/1	0.93	0.13	51,51,51,51	0
58	MG	1A	3643	1/1	0.93	0.14	21,21,21,21	0
58	MG	2A	3175	1/1	0.93	0.26	47,47,47,47	0
58	MG	1x	101	1/1	0.93	0.32	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3587	1/1	0.93	0.17	56,56,56,56	0
58	MG	2A	3845	1/1	0.93	0.14	36,36,36,36	0
58	MG	1A	3730	1/1	0.93	0.20	41,41,41,41	0
58	MG	1a	1684	1/1	0.93	0.09	37,37,37,37	0
58	MG	2A	3180	1/1	0.93	0.23	55,55,55,55	0
58	MG	1O	204	1/1	0.93	0.20	66,66,66,66	0
58	MG	1A	3731	1/1	0.93	0.21	32,32,32,32	0
58	MG	2A	3855	1/1	0.93	0.15	47,47,47,47	0
58	MG	1Q	202	1/1	0.93	0.23	31,31,31,31	0
58	MG	1A	3285	1/1	0.93	0.18	29,29,29,29	0
58	MG	1A	4052	1/1	0.93	0.27	26,26,26,26	0
58	MG	2A	3862	1/1	0.93	0.36	44,44,44,44	0
58	MG	1S	203	1/1	0.93	0.13	54,54,54,54	0
58	MG	2A	3359	1/1	0.93	0.16	50,50,50,50	0
58	MG	1a	1696	1/1	0.93	0.15	44,44,44,44	0
58	MG	1A	4053	1/1	0.93	0.20	20,20,20,20	0
58	MG	1A	3649	1/1	0.93	0.14	38,38,38,38	0
58	MG	2a	1792	1/1	0.93	0.17	49,49,49,49	0
58	MG	2A	3365	1/1	0.93	0.10	55,55,55,55	0
58	MG	1A	3738	1/1	0.93	0.20	50,50,50,50	0
58	MG	1A	3650	1/1	0.93	0.18	35,35,35,35	0
58	MG	1X	101	1/1	0.93	0.31	37,37,37,37	0
58	MG	1A	3745	1/1	0.93	0.12	53,53,53,53	0
58	MG	2A	3373	1/1	0.93	0.16	39,39,39,39	0
58	MG	2A	3194	1/1	0.93	0.31	52,52,52,52	0
58	MG	1A	3463	1/1	0.93	0.29	44,44,44,44	0
58	MG	1A	3967	1/1	0.93	0.15	35,35,35,35	0
58	MG	2A	3017	1/1	0.93	0.47	48,48,48,48	0
58	MG	1A	3304	1/1	0.93	0.23	16,16,16,16	0
58	MG	2a	1819	1/1	0.93	0.14	62,62,62,62	0
58	MG	1Z	301	1/1	0.93	0.18	59,59,59,59	0
58	MG	2A	3629	1/1	0.93	0.35	55,55,55,55	0
58	MG	2a	1827	1/1	0.93	0.23	49,49,49,49	0
58	MG	2A	3381	1/1	0.93	0.28	28,28,28,28	0
58	MG	1A	3971	1/1	0.93	0.13	28,28,28,28	0
58	MG	1A	3356	1/1	0.93	0.11	47,47,47,47	0
58	MG	1a	1723	1/1	0.93	0.33	60,60,60,60	0
58	MG	2d	302	1/1	0.93	0.16	58,58,58,58	0
58	MG	2A	3386	1/1	0.93	0.20	54,54,54,54	0
58	MG	2E	307	1/1	0.93	0.12	46,46,46,46	0
58	MG	1A	4074	1/1	0.93	0.18	21,21,21,21	0
58	MG	1A	3018	1/1	0.93	0.28	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3390	1/1	0.93	0.29	43,43,43,43	0
58	MG	1A	3979	1/1	0.93	0.10	37,37,37,37	0
58	MG	2O	201	1/1	0.93	0.21	57,57,57,57	0
58	MG	1A	3572	1/1	0.93	0.19	20,20,20,20	0
58	MG	2A	3651	1/1	0.93	0.09	49,49,49,49	0
58	MG	1A	3752	1/1	0.93	0.06	46,46,46,46	0
58	MG	2r	101	1/1	0.93	0.22	44,44,44,44	0
58	MG	1A	3755	1/1	0.93	0.20	17,17,17,17	0
58	MG	2v	101	1/1	0.93	0.31	52,52,52,52	0
58	MG	1A	3573	1/1	0.93	0.23	11,11,11,11	0
58	MG	1A	3661	1/1	0.93	0.16	54,54,54,54	0
58	MG	2A	3222	1/1	0.93	0.32	50,50,50,50	0
58	MG	2W	201	1/1	0.93	0.16	59,59,59,59	0
58	MG	2A	3403	1/1	0.93	0.15	49,49,49,49	0
58	MG	2A	3664	1/1	0.93	0.18	62,62,62,62	0
58	MG	2x	102	1/1	0.93	0.38	38,38,38,38	0
58	MG	1a	1734	1/1	0.93	0.16	37,37,37,37	0
58	MG	13	101	1/1	0.93	0.15	40,40,40,40	0
58	MG	2A	3668	1/1	0.93	0.16	52,52,52,52	0
60	ZN	14	102	1/1	0.93	0.05	80,80,80,80	0
58	MG	2A	3048	1/1	0.93	0.15	45,45,45,45	0
58	MG	1A	3772	1/1	0.93	0.15	34,34,34,34	0
58	MG	2A	3411	1/1	0.93	0.16	59,59,59,59	0
58	MG	1B	237	1/1	0.94	0.09	33,33,33,33	0
58	MG	1A	3862	1/1	0.94	0.14	34,34,34,34	0
58	MG	2A	3857	1/1	0.94	0.14	56,56,56,56	0
58	MG	2A	3858	1/1	0.94	0.12	53,53,53,53	0
58	MG	1A	3618	1/1	0.94	0.22	28,28,28,28	0
58	MG	2A	3254	1/1	0.94	0.13	50,50,50,50	0
58	MG	2A	3021	1/1	0.94	0.24	22,22,22,22	0
58	MG	1D	306	1/1	0.94	0.23	35,35,35,35	0
58	MG	1D	307	1/1	0.94	0.14	34,34,34,34	0
58	MG	1D	308	1/1	0.94	0.32	26,26,26,26	0
58	MG	2A	3027	1/1	0.94	0.19	32,32,32,32	0
58	MG	1D	309	1/1	0.94	0.19	30,30,30,30	0
58	MG	1A	3121	1/1	0.94	0.21	28,28,28,28	0
58	MG	2B	205	1/1	0.94	0.11	53,53,53,53	0
58	MG	1E	301	1/1	0.94	0.22	28,28,28,28	0
58	MG	1E	302	1/1	0.94	0.13	28,28,28,28	0
58	MG	1E	306	1/1	0.94	0.26	53,53,53,53	0
58	MG	1A	3456	1/1	0.94	0.12	31,31,31,31	0
58	MG	2A	3270	1/1	0.94	0.23	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3256	1/1	0.94	0.11	39,39,39,39	0
58	MG	1A	3739	1/1	0.94	0.08	54,54,54,54	0
58	MG	2A	3542	1/1	0.94	0.27	53,53,53,53	0
58	MG	1a	1691	1/1	0.94	0.27	41,41,41,41	0
58	MG	2B	217	1/1	0.94	0.17	46,46,46,46	0
58	MG	1A	3743	1/1	0.94	0.17	19,19,19,19	0
58	MG	2A	3276	1/1	0.94	0.15	52,52,52,52	0
58	MG	2A	3550	1/1	0.94	0.18	41,41,41,41	0
58	MG	1A	3165	1/1	0.94	0.16	42,42,42,42	0
58	MG	1A	3316	1/1	0.94	0.24	46,46,46,46	0
58	MG	1A	3746	1/1	0.94	0.29	52,52,52,52	0
58	MG	2A	3052	1/1	0.94	0.18	55,55,55,55	0
58	MG	1A	3880	1/1	0.94	0.07	48,48,48,48	0
58	MG	1A	3260	1/1	0.94	0.20	29,29,29,29	0
58	MG	2F	301	1/1	0.94	0.21	36,36,36,36	0
58	MG	2A	3286	1/1	0.94	0.27	49,49,49,49	0
58	MG	1A	3208	1/1	0.94	0.17	51,51,51,51	0
58	MG	1A	3530	1/1	0.94	0.17	45,45,45,45	0
58	MG	2F	306	1/1	0.94	0.13	40,40,40,40	0
58	MG	2A	3290	1/1	0.94	0.13	53,53,53,53	0
58	MG	1A	3321	1/1	0.94	0.14	19,19,19,19	0
58	MG	2A	3574	1/1	0.94	0.10	42,42,42,42	0
58	MG	2Q	201	1/1	0.94	0.21	46,46,46,46	0
58	MG	2R	201	1/1	0.94	0.17	60,60,60,60	0
58	MG	2A	3575	1/1	0.94	0.20	42,42,42,42	0
58	MG	1a	1705	1/1	0.94	0.23	46,46,46,46	0
58	MG	2A	3060	1/1	0.94	0.16	42,42,42,42	0
58	MG	1A	3534	1/1	0.94	0.18	30,30,30,30	0
58	MG	1a	1707	1/1	0.94	0.10	48,48,48,48	0
58	MG	2A	3298	1/1	0.94	0.16	41,41,41,41	0
58	MG	1A	3642	1/1	0.94	0.14	16,16,16,16	0
58	MG	1A	3893	1/1	0.94	0.11	31,31,31,31	0
58	MG	1A	3390	1/1	0.94	0.19	33,33,33,33	0
58	MG	2A	3589	1/1	0.94	0.19	37,37,37,37	0
58	MG	2A	3590	1/1	0.94	0.29	51,51,51,51	0
58	MG	2A	3591	1/1	0.94	0.24	38,38,38,38	0
58	MG	1A	3262	1/1	0.94	0.25	32,32,32,32	0
58	MG	2A	3068	1/1	0.94	0.30	34,34,34,34	0
58	MG	25	102	1/1	0.94	0.24	48,48,48,48	0
58	MG	25	105	1/1	0.94	0.18	45,45,45,45	0
58	MG	1a	1716	1/1	0.94	0.32	39,39,39,39	0
58	MG	1A	3759	1/1	0.94	0.11	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3897	1/1	0.94	0.20	21,21,21,21	0
58	MG	1a	1721	1/1	0.94	0.16	57,57,57,57	0
58	MG	1A	3648	1/1	0.94	0.13	40,40,40,40	0
58	MG	1A	3769	1/1	0.94	0.23	34,34,34,34	0
58	MG	2A	3601	1/1	0.94	0.21	42,42,42,42	0
58	MG	1A	3900	1/1	0.94	0.24	20,20,20,20	0
58	MG	1S	202	1/1	0.94	0.17	38,38,38,38	0
58	MG	2A	3606	1/1	0.94	0.12	66,66,66,66	0
58	MG	2A	3080	1/1	0.94	0.09	41,41,41,41	0
58	MG	2A	3608	1/1	0.94	0.38	50,50,50,50	0
58	MG	1A	3770	1/1	0.94	0.21	15,15,15,15	0
58	MG	1T	201	1/1	0.94	0.17	39,39,39,39	0
58	MG	2a	1610	1/1	0.94	0.14	47,47,47,47	0
58	MG	1A	3906	1/1	0.94	0.11	27,27,27,27	0
58	MG	2a	1613	1/1	0.94	0.34	63,63,63,63	0
58	MG	2A	3318	1/1	0.94	0.22	44,44,44,44	0
58	MG	1U	204	1/1	0.94	0.26	33,33,33,33	0
58	MG	1A	3468	1/1	0.94	0.21	25,25,25,25	0
58	MG	2A	3617	1/1	0.94	0.13	31,31,31,31	0
58	MG	2A	3089	1/1	0.94	0.25	45,45,45,45	0
58	MG	2a	1620	1/1	0.94	0.22	58,58,58,58	0
58	MG	2A	3092	1/1	0.94	0.17	31,31,31,31	0
58	MG	2a	1623	1/1	0.94	0.17	57,57,57,57	0
58	MG	1A	3063	1/1	0.94	0.35	49,49,49,49	0
58	MG	2A	3326	1/1	0.94	0.19	45,45,45,45	0
58	MG	2A	3328	1/1	0.94	0.42	64,64,64,64	0
58	MG	1W	201	1/1	0.94	0.34	41,41,41,41	0
58	MG	1A	3913	1/1	0.94	0.06	44,44,44,44	0
58	MG	1W	203	1/1	0.94	0.19	23,23,23,23	0
58	MG	1A	3127	1/1	0.94	0.22	26,26,26,26	0
58	MG	1A	3213	1/1	0.94	0.24	33,33,33,33	0
58	MG	1X	104	1/1	0.94	0.13	38,38,38,38	0
58	MG	2A	3335	1/1	0.94	0.21	32,32,32,32	0
58	MG	2A	3637	1/1	0.94	0.19	32,32,32,32	0
58	MG	1A	3776	1/1	0.94	0.13	25,25,25,25	0
58	MG	1A	3064	1/1	0.94	0.24	45,45,45,45	0
58	MG	1A	3332	1/1	0.94	0.19	48,48,48,48	0
58	MG	1A	3554	1/1	0.94	0.10	48,48,48,48	0
58	MG	1A	3477	1/1	0.94	0.21	41,41,41,41	0
58	MG	2A	3343	1/1	0.94	0.29	50,50,50,50	0
58	MG	1A	4047	1/1	0.94	0.15	25,25,25,25	0
58	MG	1A	3923	1/1	0.94	0.20	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3346	1/1	0.94	0.17	57,57,57,57	0
58	MG	1A	3478	1/1	0.94	0.19	42,42,42,42	0
58	MG	2a	1654	1/1	0.94	0.23	54,54,54,54	0
58	MG	2a	1656	1/1	0.94	0.28	50,50,50,50	0
58	MG	2a	1657	1/1	0.94	0.11	66,66,66,66	0
58	MG	1a	1749	1/1	0.94	0.24	66,66,66,66	0
58	MG	1A	3930	1/1	0.94	0.18	47,47,47,47	0
58	MG	1A	3403	1/1	0.94	0.19	30,30,30,30	0
58	MG	1a	1757	1/1	0.94	0.26	43,43,43,43	0
58	MG	2A	3120	1/1	0.94	0.17	47,47,47,47	0
58	MG	2A	3122	1/1	0.94	0.33	46,46,46,46	0
58	MG	1a	1758	1/1	0.94	0.10	49,49,49,49	0
58	MG	11	103	1/1	0.94	0.17	33,33,33,33	0
58	MG	1A	3404	1/1	0.94	0.22	39,39,39,39	0
58	MG	2a	1670	1/1	0.94	0.31	36,36,36,36	0
58	MG	2a	1672	1/1	0.94	0.18	59,59,59,59	0
58	MG	11	105	1/1	0.94	0.11	57,57,57,57	0
58	MG	1A	3564	1/1	0.94	0.19	26,26,26,26	0
58	MG	1A	3169	1/1	0.94	0.22	23,23,23,23	0
58	MG	2a	1677	1/1	0.94	0.18	41,41,41,41	0
58	MG	2A	3676	1/1	0.94	0.32	45,45,45,45	0
58	MG	2A	3134	1/1	0.94	0.20	43,43,43,43	0
58	MG	1A	3408	1/1	0.94	0.14	41,41,41,41	0
58	MG	2A	3364	1/1	0.94	0.18	52,52,52,52	0
58	MG	1A	3671	1/1	0.94	0.22	17,17,17,17	0
58	MG	1A	3939	1/1	0.94	0.16	43,43,43,43	0
58	MG	2a	1686	1/1	0.94	0.14	52,52,52,52	0
58	MG	13	106	1/1	0.94	0.15	42,42,42,42	0
58	MG	2A	3368	1/1	0.94	0.16	58,58,58,58	0
58	MG	1A	4066	1/1	0.94	0.13	46,46,46,46	0
58	MG	1A	3131	1/1	0.94	0.13	56,56,56,56	0
58	MG	1A	3416	1/1	0.94	0.28	30,30,30,30	0
58	MG	2A	3148	1/1	0.94	0.31	36,36,36,36	0
58	MG	2A	3692	1/1	0.94	0.25	51,51,51,51	0
58	MG	2a	1697	1/1	0.94	0.23	57,57,57,57	0
58	MG	16	102	1/1	0.94	0.26	46,46,46,46	0
58	MG	2a	1702	1/1	0.94	0.20	53,53,53,53	0
58	MG	17	101	1/1	0.94	0.18	23,23,23,23	0
58	MG	1A	3068	1/1	0.94	0.19	23,23,23,23	0
58	MG	18	101	1/1	0.94	0.20	39,39,39,39	0
58	MG	2a	1709	1/1	0.94	0.06	54,54,54,54	0
58	MG	1A	3222	1/1	0.94	0.22	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3223	1/1	0.94	0.16	31,31,31,31	0
58	MG	2A	3382	1/1	0.94	0.33	53,53,53,53	0
58	MG	1A	3343	1/1	0.94	0.12	24,24,24,24	0
58	MG	1a	1788	1/1	0.94	0.19	46,46,46,46	0
58	MG	1A	3069	1/1	0.94	0.18	36,36,36,36	0
58	MG	1A	3013	1/1	0.94	0.18	22,22,22,22	0
58	MG	2A	3167	1/1	0.94	0.22	36,36,36,36	0
58	MG	2A	3711	1/1	0.94	0.22	59,59,59,59	0
58	MG	1A	3688	1/1	0.94	0.19	19,19,19,19	0
58	MG	1A	3290	1/1	0.94	0.17	33,33,33,33	0
58	MG	2A	3170	1/1	0.94	0.12	53,53,53,53	0
58	MG	1A	3808	1/1	0.94	0.18	22,22,22,22	0
58	MG	2A	3393	1/1	0.94	0.10	52,52,52,52	0
58	MG	2A	3174	1/1	0.94	0.32	48,48,48,48	0
58	MG	2A	3395	1/1	0.94	0.11	42,42,42,42	0
58	MG	2a	1729	1/1	0.94	0.30	43,43,43,43	0
58	MG	2A	3396	1/1	0.94	0.28	32,32,32,32	0
58	MG	2a	1731	1/1	0.94	0.11	53,53,53,53	0
58	MG	1a	1606	1/1	0.94	0.15	41,41,41,41	0
58	MG	2a	1733	1/1	0.94	0.12	42,42,42,42	0
58	MG	1A	3182	1/1	0.94	0.14	29,29,29,29	0
58	MG	1a	1609	1/1	0.94	0.33	44,44,44,44	0
58	MG	1A	3586	1/1	0.94	0.18	20,20,20,20	0
58	MG	1A	3956	1/1	0.94	0.59	54,54,54,54	0
58	MG	1A	4095	1/1	0.94	0.09	65,65,65,65	0
58	MG	2A	3405	1/1	0.94	0.11	54,54,54,54	0
58	MG	1A	3813	1/1	0.94	0.10	43,43,43,43	0
58	MG	1A	3054	1/1	0.94	0.08	32,32,32,32	0
58	MG	2a	1746	1/1	0.94	0.32	69,69,69,69	0
58	MG	1a	1804	1/1	0.94	0.20	43,43,43,43	0
58	MG	1a	1617	1/1	0.94	0.16	40,40,40,40	0
58	MG	1A	3590	1/1	0.94	0.26	36,36,36,36	0
58	MG	2A	3414	1/1	0.94	0.36	59,59,59,59	0
58	MG	1A	3591	1/1	0.94	0.21	24,24,24,24	0
58	MG	1A	3146	1/1	0.94	0.15	29,29,29,29	0
58	MG	1A	3823	1/1	0.94	0.16	27,27,27,27	0
58	MG	1A	4105	1/1	0.94	0.15	42,42,42,42	0
58	MG	1A	3965	1/1	0.94	0.10	31,31,31,31	0
58	MG	2A	3422	1/1	0.94	0.31	35,35,35,35	0
58	MG	2A	3753	1/1	0.94	0.16	58,58,58,58	0
58	MG	1A	3594	1/1	0.94	0.16	34,34,34,34	0
58	MG	1A	3017	1/1	0.94	0.15	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2a	1764	1/1	0.94	0.15	50,50,50,50	0
58	MG	1d	301	1/1	0.94	0.28	59,59,59,59	0
58	MG	1A	3111	1/1	0.94	0.15	34,34,34,34	0
58	MG	2A	3432	1/1	0.94	0.41	46,46,46,46	0
58	MG	2A	3196	1/1	0.94	0.40	36,36,36,36	0
58	MG	2A	3198	1/1	0.94	0.37	56,56,56,56	0
58	MG	1A	3972	1/1	0.94	0.10	61,61,61,61	0
58	MG	2a	1773	1/1	0.94	0.13	50,50,50,50	0
58	MG	2A	3765	1/1	0.94	0.14	56,56,56,56	0
58	MG	2A	3436	1/1	0.94	0.27	48,48,48,48	0
58	MG	1l	201	1/1	0.94	0.18	49,49,49,49	0
58	MG	2A	3201	1/1	0.94	0.15	51,51,51,51	0
58	MG	1A	3703	1/1	0.94	0.19	25,25,25,25	0
58	MG	1A	3832	1/1	0.94	0.20	18,18,18,18	0
58	MG	2A	3444	1/1	0.94	0.18	58,58,58,58	0
58	MG	2A	3778	1/1	0.94	0.13	46,46,46,46	0
58	MG	2A	3204	1/1	0.94	0.10	48,48,48,48	0
58	MG	1n	101	1/1	0.94	0.23	58,58,58,58	0
58	MG	1B	207	1/1	0.94	0.20	50,50,50,50	0
58	MG	1a	1640	1/1	0.94	0.20	47,47,47,47	0
58	MG	1A	3704	1/1	0.94	0.12	48,48,48,48	0
58	MG	2a	1797	1/1	0.94	0.20	50,50,50,50	0
58	MG	2a	1798	1/1	0.94	0.21	51,51,51,51	0
58	MG	2A	3211	1/1	0.94	0.22	41,41,41,41	0
58	MG	1A	3504	1/1	0.94	0.19	30,30,30,30	0
58	MG	2a	1802	1/1	0.94	0.09	66,66,66,66	0
58	MG	2a	1803	1/1	0.94	0.14	58,58,58,58	0
58	MG	1w	108	1/1	0.94	0.16	33,33,33,33	0
58	MG	1A	3984	1/1	0.94	0.14	49,49,49,49	0
58	MG	2A	3791	1/1	0.94	0.09	57,57,57,57	0
58	MG	2A	3796	1/1	0.94	0.18	33,33,33,33	0
58	MG	2A	3460	1/1	0.94	0.41	40,40,40,40	0
58	MG	2a	1812	1/1	0.94	0.08	58,58,58,58	0
58	MG	2a	1813	1/1	0.94	0.16	59,59,59,59	0
58	MG	2A	3462	1/1	0.94	0.17	45,45,45,45	0
58	MG	1A	3187	1/1	0.94	0.17	28,28,28,28	0
58	MG	1B	215	1/1	0.94	0.15	39,39,39,39	0
58	MG	2a	1818	1/1	0.94	0.18	61,61,61,61	0
58	MG	1A	3151	1/1	0.94	0.22	22,22,22,22	0
58	MG	2A	3220	1/1	0.94	0.25	40,40,40,40	0
58	MG	1B	218	1/1	0.94	0.21	42,42,42,42	0
58	MG	2A	3474	1/1	0.94	0.32	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3808	1/1	0.94	0.15	36,36,36,36	0
58	MG	1A	3059	1/1	0.94	0.26	30,30,30,30	0
58	MG	1B	221	1/1	0.94	0.19	25,25,25,25	0
58	MG	1A	3849	1/1	0.94	0.15	54,54,54,54	0
58	MG	1a	1655	1/1	0.94	0.22	39,39,39,39	0
58	MG	2f	201	1/1	0.94	0.23	38,38,38,38	0
58	MG	2A	3484	1/1	0.94	0.16	52,52,52,52	0
58	MG	2A	3816	1/1	0.94	0.19	49,49,49,49	0
58	MG	2A	3817	1/1	0.94	0.17	35,35,35,35	0
58	MG	1A	3444	1/1	0.94	0.15	39,39,39,39	0
58	MG	2A	3490	1/1	0.94	0.23	34,34,34,34	0
58	MG	1x	110	1/1	0.94	0.29	67,67,67,67	0
58	MG	2A	3229	1/1	0.94	0.22	44,44,44,44	0
58	MG	2A	3493	1/1	0.94	0.30	32,32,32,32	0
58	MG	2A	3829	1/1	0.94	0.27	37,37,37,37	0
58	MG	2p	101	1/1	0.94	0.08	58,58,58,58	0
58	MG	1A	3991	1/1	0.94	0.20	60,60,60,60	0
58	MG	2A	3002	1/1	0.94	0.42	52,52,52,52	0
58	MG	2A	3834	1/1	0.94	0.25	24,24,24,24	0
58	MG	2A	3836	1/1	0.94	0.20	37,37,37,37	0
58	MG	2A	3003	1/1	0.94	0.28	45,45,45,45	0
58	MG	1A	3251	1/1	0.94	0.19	47,47,47,47	0
58	MG	2v	104	1/1	0.94	0.17	59,59,59,59	0
58	MG	1A	3449	1/1	0.94	0.24	35,35,35,35	0
58	MG	2A	3500	1/1	0.94	0.29	47,47,47,47	0
58	MG	1A	3001	1/1	0.94	0.20	36,36,36,36	0
58	MG	2A	3007	1/1	0.94	0.16	34,34,34,34	0
58	MG	2A	3503	1/1	0.94	0.24	42,42,42,42	0
58	MG	1a	1663	1/1	0.94	0.17	53,53,53,53	0
58	MG	1A	3194	1/1	0.94	0.16	29,29,29,29	0
58	MG	2A	3847	1/1	0.94	0.16	29,29,29,29	0
58	MG	2x	107	1/1	0.94	0.31	45,45,45,45	0
58	MG	2y	101	1/1	0.94	0.17	61,61,61,61	0
58	MG	1A	3519	1/1	0.94	0.20	23,23,23,23	0
58	MG	2A	3245	1/1	0.94	0.26	35,35,35,35	0
58	MG	1A	3999	1/1	0.94	0.11	20,20,20,20	0
58	MG	2A	3248	1/1	0.94	0.23	46,46,46,46	0
58	MG	1A	3007	1/1	0.95	0.14	20,20,20,20	0
58	MG	1a	1755	1/1	0.95	0.17	43,43,43,43	0
58	MG	1a	1756	1/1	0.95	0.13	45,45,45,45	0
58	MG	2A	3339	1/1	0.95	0.28	48,48,48,48	0
58	MG	1A	3419	1/1	0.95	0.18	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2Q	202	1/1	0.95	0.31	46,46,46,46	0
58	MG	1A	3753	1/1	0.95	0.24	15,15,15,15	0
58	MG	1a	1759	1/1	0.95	0.12	49,49,49,49	0
58	MG	1A	3333	1/1	0.95	0.34	37,37,37,37	0
58	MG	2A	3125	1/1	0.95	0.10	43,43,43,43	0
58	MG	1A	3155	1/1	0.95	0.24	34,34,34,34	0
58	MG	1A	4056	1/1	0.95	0.20	34,34,34,34	0
58	MG	2A	3128	1/1	0.95	0.24	45,45,45,45	0
58	MG	2A	3616	1/1	0.95	0.26	43,43,43,43	0
58	MG	2A	3130	1/1	0.95	0.21	44,44,44,44	0
58	MG	1A	4057	1/1	0.95	0.20	22,22,22,22	0
58	MG	2Z	301	1/1	0.95	0.12	62,62,62,62	0
58	MG	1a	1765	1/1	0.95	0.12	38,38,38,38	0
58	MG	1A	3114	1/1	0.95	0.24	26,26,26,26	0
58	MG	1A	4059	1/1	0.95	0.12	41,41,41,41	0
58	MG	1A	4061	1/1	0.95	0.29	57,57,57,57	0
58	MG	1A	3762	1/1	0.95	0.13	51,51,51,51	0
58	MG	1a	1771	1/1	0.95	0.30	57,57,57,57	0
58	MG	25	104	1/1	0.95	0.27	48,48,48,48	0
58	MG	2A	3141	1/1	0.95	0.20	50,50,50,50	0
58	MG	2A	3142	1/1	0.95	0.30	47,47,47,47	0
58	MG	1A	3764	1/1	0.95	0.21	39,39,39,39	0
58	MG	2A	3632	1/1	0.95	0.30	32,32,32,32	0
58	MG	2A	3633	1/1	0.95	0.10	61,61,61,61	0
58	MG	15	101	1/1	0.95	0.18	24,24,24,24	0
58	MG	15	105	1/1	0.95	0.20	23,23,23,23	0
58	MG	1A	4064	1/1	0.95	0.19	40,40,40,40	0
58	MG	1a	1776	1/1	0.95	0.09	40,40,40,40	0
58	MG	1a	1777	1/1	0.95	0.12	58,58,58,58	0
58	MG	2A	3644	1/1	0.95	0.26	50,50,50,50	0
58	MG	2A	3153	1/1	0.95	0.19	40,40,40,40	0
58	MG	1A	3766	1/1	0.95	0.21	20,20,20,20	0
58	MG	16	101	1/1	0.95	0.73	60,60,60,60	0
58	MG	1A	3622	1/1	0.95	0.17	42,42,42,42	0
58	MG	1a	1781	1/1	0.95	0.16	36,36,36,36	0
58	MG	2a	1611	1/1	0.95	0.10	51,51,51,51	0
58	MG	1A	3924	1/1	0.95	0.18	27,27,27,27	0
58	MG	1A	3925	1/1	0.95	0.16	31,31,31,31	0
58	MG	17	105	1/1	0.95	0.22	28,28,28,28	0
58	MG	2a	1615	1/1	0.95	0.17	54,54,54,54	0
58	MG	1A	3511	1/1	0.95	0.15	41,41,41,41	0
58	MG	1A	3929	1/1	0.95	0.20	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3625	1/1	0.95	0.17	31,31,31,31	0
58	MG	1A	4075	1/1	0.95	0.15	46,46,46,46	0
58	MG	2A	3663	1/1	0.95	0.30	50,50,50,50	0
58	MG	1A	3116	1/1	0.95	0.23	29,29,29,29	0
58	MG	2a	1622	1/1	0.95	0.24	62,62,62,62	0
58	MG	1A	3053	1/1	0.95	0.12	32,32,32,32	0
58	MG	1A	4082	1/1	0.95	0.16	31,31,31,31	0
58	MG	1A	3630	1/1	0.95	0.22	28,28,28,28	0
58	MG	2A	3669	1/1	0.95	0.20	32,32,32,32	0
58	MG	1A	3338	1/1	0.95	0.31	46,46,46,46	0
58	MG	2a	1630	1/1	0.95	0.34	57,57,57,57	0
58	MG	1A	3633	1/1	0.95	0.22	19,19,19,19	0
58	MG	1A	4089	1/1	0.95	0.13	48,48,48,48	0
58	MG	1A	3636	1/1	0.95	0.18	36,36,36,36	0
58	MG	1A	3518	1/1	0.95	0.14	46,46,46,46	0
58	MG	1A	3119	1/1	0.95	0.22	27,27,27,27	0
58	MG	1A	3341	1/1	0.95	0.28	48,48,48,48	0
58	MG	1A	3089	1/1	0.95	0.14	41,41,41,41	0
58	MG	1a	1805	1/1	0.95	0.26	52,52,52,52	0
58	MG	1A	3277	1/1	0.95	0.22	34,34,34,34	0
58	MG	1A	3281	1/1	0.95	0.12	24,24,24,24	0
58	MG	1A	3283	1/1	0.95	0.13	24,24,24,24	0
58	MG	1a	1620	1/1	0.95	0.21	46,46,46,46	0
58	MG	2A	3686	1/1	0.95	0.16	38,38,38,38	0
58	MG	2A	3687	1/1	0.95	0.20	50,50,50,50	0
58	MG	1A	3350	1/1	0.95	0.29	54,54,54,54	0
58	MG	1A	3949	1/1	0.95	0.07	36,36,36,36	0
58	MG	1A	3353	1/1	0.95	0.43	48,48,48,48	0
58	MG	1A	3122	1/1	0.95	0.18	32,32,32,32	0
58	MG	2a	1655	1/1	0.95	0.13	58,58,58,58	0
58	MG	1a	1625	1/1	0.95	0.27	48,48,48,48	0
58	MG	1A	3531	1/1	0.95	0.20	41,41,41,41	0
58	MG	1A	3123	1/1	0.95	0.19	32,32,32,32	0
58	MG	2A	3409	1/1	0.95	0.09	58,58,58,58	0
58	MG	1a	1628	1/1	0.95	0.30	46,46,46,46	0
58	MG	2A	3197	1/1	0.95	0.16	48,48,48,48	0
58	MG	1f	201	1/1	0.95	0.33	43,43,43,43	0
58	MG	2A	3413	1/1	0.95	0.18	54,54,54,54	0
58	MG	2a	1665	1/1	0.95	0.22	55,55,55,55	0
58	MG	1A	3357	1/1	0.95	0.27	60,60,60,60	0
58	MG	1A	3536	1/1	0.95	0.22	46,46,46,46	0
58	MG	2A	3416	1/1	0.95	0.23	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3417	1/1	0.95	0.20	48,48,48,48	0
58	MG	2a	1671	1/1	0.95	0.19	53,53,53,53	0
58	MG	1a	1631	1/1	0.95	0.16	44,44,44,44	0
58	MG	1A	3124	1/1	0.95	0.35	46,46,46,46	0
58	MG	1a	1634	1/1	0.95	0.30	22,22,22,22	0
58	MG	1A	3538	1/1	0.95	0.27	36,36,36,36	0
58	MG	2a	1676	1/1	0.95	0.24	44,44,44,44	0
58	MG	1a	1636	1/1	0.95	0.20	62,62,62,62	0
58	MG	1A	3091	1/1	0.95	0.21	42,42,42,42	0
58	MG	2a	1679	1/1	0.95	0.12	42,42,42,42	0
58	MG	1B	205	1/1	0.95	0.14	40,40,40,40	0
58	MG	1A	3540	1/1	0.95	0.30	32,32,32,32	0
58	MG	2A	3210	1/1	0.95	0.14	51,51,51,51	0
58	MG	2A	3431	1/1	0.95	0.36	49,49,49,49	0
58	MG	1A	3009	1/1	0.95	0.18	19,19,19,19	0
58	MG	1A	3962	1/1	0.95	0.12	38,38,38,38	0
58	MG	2A	3724	1/1	0.95	0.12	53,53,53,53	0
58	MG	1A	3664	1/1	0.95	0.14	37,37,37,37	0
58	MG	1A	3543	1/1	0.95	0.28	43,43,43,43	0
58	MG	2A	3729	1/1	0.95	0.30	46,46,46,46	0
58	MG	1A	3809	1/1	0.95	0.20	13,13,13,13	0
58	MG	1A	3966	1/1	0.95	0.18	44,44,44,44	0
58	MG	2a	1693	1/1	0.95	0.19	48,48,48,48	0
58	MG	1B	217	1/1	0.95	0.13	58,58,58,58	0
58	MG	2a	1696	1/1	0.95	0.21	43,43,43,43	0
58	MG	2A	3734	1/1	0.95	0.27	36,36,36,36	0
58	MG	1A	3228	1/1	0.95	0.26	39,39,39,39	0
58	MG	2a	1699	1/1	0.95	0.10	52,52,52,52	0
58	MG	2a	1701	1/1	0.95	0.38	54,54,54,54	0
58	MG	2A	3737	1/1	0.95	0.17	57,57,57,57	0
58	MG	2A	3738	1/1	0.95	0.14	46,46,46,46	0
58	MG	1A	3174	1/1	0.95	0.17	36,36,36,36	0
58	MG	2a	1705	1/1	0.95	0.33	56,56,56,56	0
58	MG	1A	3970	1/1	0.95	0.08	41,41,41,41	0
58	MG	2a	1708	1/1	0.95	0.10	52,52,52,52	0
58	MG	1B	223	1/1	0.95	0.25	40,40,40,40	0
58	MG	1A	3549	1/1	0.95	0.19	52,52,52,52	0
58	MG	1A	3294	1/1	0.95	0.18	25,25,25,25	0
58	MG	1A	3233	1/1	0.95	0.15	40,40,40,40	0
58	MG	1A	3975	1/1	0.95	0.20	16,16,16,16	0
58	MG	1A	3976	1/1	0.95	0.15	37,37,37,37	0
58	MG	2A	3748	1/1	0.95	0.30	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3235	1/1	0.95	0.19	53,53,53,53	0
58	MG	2a	1719	1/1	0.95	0.11	68,68,68,68	0
58	MG	2A	3750	1/1	0.95	0.35	65,65,65,65	0
58	MG	2A	3751	1/1	0.95	0.30	56,56,56,56	0
58	MG	2A	3455	1/1	0.95	0.45	47,47,47,47	0
58	MG	1A	3066	1/1	0.95	0.28	34,34,34,34	0
58	MG	1A	3980	1/1	0.95	0.11	52,52,52,52	0
58	MG	2A	3459	1/1	0.95	0.22	63,63,63,63	0
58	MG	1A	3301	1/1	0.95	0.40	57,57,57,57	0
58	MG	1A	3464	1/1	0.95	0.23	38,38,38,38	0
58	MG	1A	3029	1/1	0.95	0.18	23,23,23,23	0
58	MG	2A	3464	1/1	0.95	0.28	31,31,31,31	0
58	MG	1D	301	1/1	0.95	0.22	47,47,47,47	0
58	MG	2A	3762	1/1	0.95	0.14	46,46,46,46	0
58	MG	1A	3467	1/1	0.95	0.14	51,51,51,51	0
58	MG	1A	3376	1/1	0.95	0.23	41,41,41,41	0
58	MG	1A	3056	1/1	0.95	0.26	32,32,32,32	0
58	MG	1A	3470	1/1	0.95	0.11	28,28,28,28	0
58	MG	2A	3246	1/1	0.95	0.22	56,56,56,56	0
58	MG	1a	1676	1/1	0.95	0.23	43,43,43,43	0
58	MG	1a	1677	1/1	0.95	0.19	37,37,37,37	0
58	MG	1A	3305	1/1	0.95	0.33	38,38,38,38	0
58	MG	2a	1742	1/1	0.95	0.20	55,55,55,55	0
58	MG	2A	3251	1/1	0.95	0.24	46,46,46,46	0
58	MG	1A	3379	1/1	0.95	0.18	29,29,29,29	0
58	MG	2a	1745	1/1	0.95	0.18	44,44,44,44	0
58	MG	1A	3381	1/1	0.95	0.18	39,39,39,39	0
58	MG	2A	3034	1/1	0.95	0.11	35,35,35,35	0
58	MG	1A	3847	1/1	0.95	0.11	30,30,30,30	0
58	MG	1A	3133	1/1	0.95	0.14	23,23,23,23	0
58	MG	1A	3384	1/1	0.95	0.19	23,23,23,23	0
58	MG	2A	3259	1/1	0.95	0.27	43,43,43,43	0
58	MG	1A	3057	1/1	0.95	0.23	31,31,31,31	0
58	MG	1A	3576	1/1	0.95	0.30	39,39,39,39	0
58	MG	2A	3789	1/1	0.95	0.17	32,32,32,32	0
58	MG	1F	302	1/1	0.95	0.26	24,24,24,24	0
58	MG	2A	3794	1/1	0.95	0.23	47,47,47,47	0
58	MG	2A	3795	1/1	0.95	0.14	38,38,38,38	0
58	MG	2A	3499	1/1	0.95	0.11	51,51,51,51	0
58	MG	1A	3387	1/1	0.95	0.19	24,24,24,24	0
58	MG	1A	3854	1/1	0.95	0.18	33,33,33,33	0
58	MG	2A	3047	1/1	0.95	0.24	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3801	1/1	0.95	0.11	59,59,59,59	0
58	MG	2A	3802	1/1	0.95	0.10	64,64,64,64	0
58	MG	1A	3856	1/1	0.95	0.15	43,43,43,43	0
58	MG	2A	3504	1/1	0.95	0.21	32,32,32,32	0
58	MG	1A	3579	1/1	0.95	0.18	30,30,30,30	0
58	MG	1A	3099	1/1	0.95	0.19	43,43,43,43	0
58	MG	1A	3144	1/1	0.95	0.09	42,42,42,42	0
58	MG	1A	3037	1/1	0.95	0.24	16,16,16,16	0
58	MG	2a	1776	1/1	0.95	0.13	49,49,49,49	0
58	MG	2A	3509	1/1	0.95	0.23	54,54,54,54	0
58	MG	2a	1778	1/1	0.95	0.17	38,38,38,38	0
58	MG	1A	3864	1/1	0.95	0.21	34,34,34,34	0
58	MG	1A	3709	1/1	0.95	0.24	20,20,20,20	0
58	MG	1A	3712	1/1	0.95	0.20	28,28,28,28	0
58	MG	2A	3277	1/1	0.95	0.19	56,56,56,56	0
58	MG	2a	1785	1/1	0.95	0.24	63,63,63,63	0
58	MG	2A	3058	1/1	0.95	0.21	46,46,46,46	0
58	MG	2A	3279	1/1	0.95	0.10	47,47,47,47	0
58	MG	2a	1788	1/1	0.95	0.17	57,57,57,57	0
58	MG	2a	1789	1/1	0.95	0.12	66,66,66,66	0
58	MG	2A	3518	1/1	0.95	0.18	25,25,25,25	0
58	MG	1A	3102	1/1	0.95	0.12	56,56,56,56	0
58	MG	1A	4017	1/1	0.95	0.11	16,16,16,16	0
58	MG	2a	1793	1/1	0.95	0.26	59,59,59,59	0
58	MG	2a	1794	1/1	0.95	0.13	51,51,51,51	0
58	MG	2A	3061	1/1	0.95	0.18	30,30,30,30	0
58	MG	1a	1709	1/1	0.95	0.15	52,52,52,52	0
58	MG	1N	204	1/1	0.95	0.12	37,37,37,37	0
58	MG	2A	3527	1/1	0.95	0.16	32,32,32,32	0
58	MG	1N	205	1/1	0.95	0.14	35,35,35,35	0
58	MG	1A	3588	1/1	0.95	0.18	29,29,29,29	0
58	MG	2A	3532	1/1	0.95	0.20	59,59,59,59	0
58	MG	1a	1714	1/1	0.95	0.22	42,42,42,42	0
58	MG	2a	1805	1/1	0.95	0.20	52,52,52,52	0
58	MG	1A	3148	1/1	0.95	0.26	24,24,24,24	0
58	MG	1A	3488	1/1	0.95	0.07	48,48,48,48	0
58	MG	2A	3292	1/1	0.95	0.39	53,53,53,53	0
58	MG	2A	3069	1/1	0.95	0.22	27,27,27,27	0
58	MG	1A	3396	1/1	0.95	0.23	29,29,29,29	0
58	MG	2A	3295	1/1	0.95	0.18	52,52,52,52	0
58	MG	2A	3071	1/1	0.95	0.22	43,43,43,43	0
58	MG	1a	1720	1/1	0.95	0.20	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3192	1/1	0.95	0.15	27,27,27,27	0
58	MG	2A	3547	1/1	0.95	0.25	51,51,51,51	0
58	MG	1Q	204	1/1	0.95	0.15	37,37,37,37	0
58	MG	1A	3193	1/1	0.95	0.13	21,21,21,21	0
58	MG	2a	1822	1/1	0.95	0.29	44,44,44,44	0
58	MG	1Q	208	1/1	0.95	0.13	33,33,33,33	0
58	MG	2A	3852	1/1	0.95	0.17	41,41,41,41	0
58	MG	1a	1725	1/1	0.95	0.15	42,42,42,42	0
58	MG	1A	3727	1/1	0.95	0.16	42,42,42,42	0
58	MG	2a	1831	1/1	0.95	0.27	55,55,55,55	0
58	MG	2A	3555	1/1	0.95	0.19	34,34,34,34	0
58	MG	2A	3557	1/1	0.95	0.20	29,29,29,29	0
58	MG	2d	301	1/1	0.95	0.28	48,48,48,48	0
58	MG	1A	3595	1/1	0.95	0.17	21,21,21,21	0
58	MG	2A	3561	1/1	0.95	0.17	43,43,43,43	0
58	MG	1A	3060	1/1	0.95	0.26	33,33,33,33	0
58	MG	2A	3082	1/1	0.95	0.12	51,51,51,51	0
58	MG	2A	3564	1/1	0.95	0.11	36,36,36,36	0
58	MG	1A	3883	1/1	0.95	0.20	33,33,33,33	0
58	MG	1T	202	1/1	0.95	0.17	37,37,37,37	0
58	MG	2A	3086	1/1	0.95	0.19	45,45,45,45	0
58	MG	1A	3401	1/1	0.95	0.17	20,20,20,20	0
58	MG	1A	3259	1/1	0.95	0.14	58,58,58,58	0
58	MG	2A	3573	1/1	0.95	0.11	30,30,30,30	0
58	MG	2A	3313	1/1	0.95	0.19	46,46,46,46	0
58	MG	1A	4032	1/1	0.95	0.15	34,34,34,34	0
58	MG	1A	3736	1/1	0.95	0.21	51,51,51,51	0
58	MG	1A	3197	1/1	0.95	0.15	27,27,27,27	0
58	MG	1A	3600	1/1	0.95	0.22	34,34,34,34	0
58	MG	1A	3740	1/1	0.95	0.15	41,41,41,41	0
58	MG	1A	3742	1/1	0.95	0.16	26,26,26,26	0
58	MG	1A	3082	1/1	0.95	0.20	34,34,34,34	0
58	MG	1A	3603	1/1	0.95	0.21	37,37,37,37	0
58	MG	1A	3407	1/1	0.95	0.19	36,36,36,36	0
58	MG	2A	3324	1/1	0.95	0.14	61,61,61,61	0
58	MG	1A	3607	1/1	0.95	0.17	53,53,53,53	0
58	MG	1A	3199	1/1	0.95	0.22	39,39,39,39	0
58	MG	2A	3327	1/1	0.95	0.22	34,34,34,34	0
58	MG	2A	3593	1/1	0.95	0.12	58,58,58,58	0
58	MG	2A	3107	1/1	0.95	0.20	52,52,52,52	0
58	MG	1A	3903	1/1	0.95	0.18	21,21,21,21	0
58	MG	1A	3112	1/1	0.95	0.15	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3330	1/1	0.95	0.16	43,43,43,43	0
58	MG	1A	3909	1/1	0.95	0.14	40,40,40,40	0
58	MG	1a	1751	1/1	0.95	0.14	45,45,45,45	0
58	MG	1A	3331	1/1	0.95	0.14	29,29,29,29	0
58	MG	2A	3604	1/1	0.96	0.17	47,47,47,47	0
58	MG	1A	3041	1/1	0.96	0.20	26,26,26,26	0
58	MG	1a	1762	1/1	0.96	0.19	41,41,41,41	0
58	MG	1A	3638	1/1	0.96	0.17	19,19,19,19	0
58	MG	2A	3123	1/1	0.96	0.14	62,62,62,62	0
58	MG	1A	3922	1/1	0.96	0.18	30,30,30,30	0
58	MG	1A	3533	1/1	0.96	0.13	32,32,32,32	0
58	MG	1A	3380	1/1	0.96	0.17	23,23,23,23	0
58	MG	1A	3065	1/1	0.96	0.21	27,27,27,27	0
58	MG	1A	4068	1/1	0.96	0.15	11,11,11,11	0
58	MG	1a	1769	1/1	0.96	0.10	35,35,35,35	0
58	MG	2U	202	1/1	0.96	0.18	36,36,36,36	0
58	MG	2V	201	1/1	0.96	0.14	45,45,45,45	0
58	MG	15	103	1/1	0.96	0.13	23,23,23,23	0
58	MG	15	104	1/1	0.96	0.13	24,24,24,24	0
58	MG	1A	3236	1/1	0.96	0.18	35,35,35,35	0
58	MG	1A	3928	1/1	0.96	0.12	25,25,25,25	0
58	MG	2Y	201	1/1	0.96	0.18	45,45,45,45	0
58	MG	2A	3620	1/1	0.96	0.15	43,43,43,43	0
58	MG	1A	3328	1/1	0.96	0.16	35,35,35,35	0
58	MG	1A	3779	1/1	0.96	0.14	33,33,33,33	0
58	MG	2A	3138	1/1	0.96	0.18	31,31,31,31	0
58	MG	1A	3931	1/1	0.96	0.13	24,24,24,24	0
58	MG	23	103	1/1	0.96	0.20	33,33,33,33	0
58	MG	2A	3361	1/1	0.96	0.24	54,54,54,54	0
58	MG	2A	3627	1/1	0.96	0.17	34,34,34,34	0
58	MG	1A	3932	1/1	0.96	0.06	49,49,49,49	0
58	MG	1A	3274	1/1	0.96	0.13	32,32,32,32	0
58	MG	1A	3276	1/1	0.96	0.18	32,32,32,32	0
58	MG	2A	3144	1/1	0.96	0.37	41,41,41,41	0
58	MG	1A	3541	1/1	0.96	0.19	40,40,40,40	0
58	MG	1A	3388	1/1	0.96	0.19	31,31,31,31	0
58	MG	1A	3785	1/1	0.96	0.17	31,31,31,31	0
58	MG	1A	3786	1/1	0.96	0.07	33,33,33,33	0
58	MG	1A	4087	1/1	0.96	0.19	40,40,40,40	0
58	MG	2A	3371	1/1	0.96	0.32	51,51,51,51	0
58	MG	2A	3642	1/1	0.96	0.13	42,42,42,42	0
58	MG	2A	3643	1/1	0.96	0.20	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3372	1/1	0.96	0.20	49,49,49,49	0
58	MG	2A	3151	1/1	0.96	0.10	54,54,54,54	0
58	MG	1a	1785	1/1	0.96	0.08	48,48,48,48	0
58	MG	1A	3176	1/1	0.96	0.19	26,26,26,26	0
58	MG	2A	3648	1/1	0.96	0.22	36,36,36,36	0
58	MG	1a	1787	1/1	0.96	0.12	46,46,46,46	0
58	MG	2A	3157	1/1	0.96	0.17	43,43,43,43	0
58	MG	1A	3940	1/1	0.96	0.17	23,23,23,23	0
58	MG	1A	3201	1/1	0.96	0.17	34,34,34,34	0
58	MG	2A	3160	1/1	0.96	0.15	55,55,55,55	0
58	MG	1A	3391	1/1	0.96	0.20	23,23,23,23	0
58	MG	2A	3656	1/1	0.96	0.16	51,51,51,51	0
58	MG	1a	1791	1/1	0.96	0.12	39,39,39,39	0
58	MG	1A	3547	1/1	0.96	0.28	40,40,40,40	0
58	MG	2A	3660	1/1	0.96	0.18	40,40,40,40	0
58	MG	2A	3661	1/1	0.96	0.14	51,51,51,51	0
58	MG	1A	3791	1/1	0.96	0.20	27,27,27,27	0
58	MG	1a	1608	1/1	0.96	0.17	43,43,43,43	0
58	MG	1A	3548	1/1	0.96	0.32	52,52,52,52	0
58	MG	2A	3388	1/1	0.96	0.12	51,51,51,51	0
58	MG	1A	3794	1/1	0.96	0.24	23,23,23,23	0
58	MG	1A	4098	1/1	0.96	0.23	45,45,45,45	0
58	MG	2a	1629	1/1	0.96	0.27	48,48,48,48	0
58	MG	1a	1798	1/1	0.96	0.12	54,54,54,54	0
58	MG	2A	3171	1/1	0.96	0.16	59,59,59,59	0
58	MG	2A	3172	1/1	0.96	0.29	39,39,39,39	0
58	MG	1A	3282	1/1	0.96	0.25	33,33,33,33	0
58	MG	1A	4100	1/1	0.96	0.25	50,50,50,50	0
58	MG	1A	3797	1/1	0.96	0.18	22,22,22,22	0
58	MG	2a	1638	1/1	0.96	0.18	45,45,45,45	0
58	MG	1a	1616	1/1	0.96	0.23	54,54,54,54	0
58	MG	2A	3398	1/1	0.96	0.11	51,51,51,51	0
58	MG	2A	3679	1/1	0.96	0.24	35,35,35,35	0
58	MG	2A	3177	1/1	0.96	0.34	39,39,39,39	0
58	MG	2A	3400	1/1	0.96	0.17	43,43,43,43	0
58	MG	1A	3239	1/1	0.96	0.18	31,31,31,31	0
58	MG	1a	1618	1/1	0.96	0.17	40,40,40,40	0
58	MG	1A	4103	1/1	0.96	0.24	51,51,51,51	0
58	MG	1A	3130	1/1	0.96	0.19	26,26,26,26	0
58	MG	1A	3552	1/1	0.96	0.16	40,40,40,40	0
58	MG	2a	1651	1/1	0.96	0.22	38,38,38,38	0
58	MG	1A	3471	1/1	0.96	0.15	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3243	1/1	0.96	0.31	37,37,37,37	0
58	MG	1A	3244	1/1	0.96	0.25	28,28,28,28	0
58	MG	2A	3690	1/1	0.96	0.14	53,53,53,53	0
58	MG	1A	3556	1/1	0.96	0.11	46,46,46,46	0
58	MG	1A	3957	1/1	0.96	0.09	39,39,39,39	0
58	MG	1A	3668	1/1	0.96	0.17	43,43,43,43	0
58	MG	1A	3670	1/1	0.96	0.23	21,21,21,21	0
58	MG	2A	3695	1/1	0.96	0.29	30,30,30,30	0
58	MG	1A	3398	1/1	0.96	0.26	40,40,40,40	0
58	MG	1A	3245	1/1	0.96	0.25	34,34,34,34	0
58	MG	1A	3810	1/1	0.96	0.18	37,37,37,37	0
58	MG	2A	3702	1/1	0.96	0.17	50,50,50,50	0
58	MG	1A	3339	1/1	0.96	0.29	41,41,41,41	0
58	MG	1k	201	1/1	0.96	0.22	41,41,41,41	0
58	MG	1A	3207	1/1	0.96	0.23	27,27,27,27	0
58	MG	1B	211	1/1	0.96	0.25	43,43,43,43	0
58	MG	1B	212	1/1	0.96	0.12	33,33,33,33	0
58	MG	1A	3565	1/1	0.96	0.20	24,24,24,24	0
58	MG	1n	102	1/1	0.96	0.18	35,35,35,35	0
58	MG	1A	3402	1/1	0.96	0.18	30,30,30,30	0
58	MG	2A	3425	1/1	0.96	0.38	38,38,38,38	0
58	MG	2A	3426	1/1	0.96	0.40	48,48,48,48	0
58	MG	1a	1639	1/1	0.96	0.13	50,50,50,50	0
58	MG	1w	104	1/1	0.96	0.40	63,63,63,63	0
58	MG	1A	3817	1/1	0.96	0.09	35,35,35,35	0
58	MG	1A	3247	1/1	0.96	0.22	31,31,31,31	0
58	MG	1A	3181	1/1	0.96	0.15	27,27,27,27	0
58	MG	2A	3719	1/1	0.96	0.13	44,44,44,44	0
58	MG	1A	3683	1/1	0.96	0.17	21,21,21,21	0
58	MG	1A	3822	1/1	0.96	0.14	22,22,22,22	0
58	MG	1B	222	1/1	0.96	0.16	52,52,52,52	0
58	MG	1A	3973	1/1	0.96	0.17	26,26,26,26	0
58	MG	1A	3484	1/1	0.96	0.20	30,30,30,30	0
58	MG	1B	226	1/1	0.96	0.18	36,36,36,36	0
58	MG	1a	1651	1/1	0.96	0.21	43,43,43,43	0
58	MG	2A	3728	1/1	0.96	0.25	35,35,35,35	0
58	MG	1B	227	1/1	0.96	0.14	49,49,49,49	0
58	MG	1A	3209	1/1	0.96	0.23	27,27,27,27	0
58	MG	1A	3406	1/1	0.96	0.17	37,37,37,37	0
58	MG	1A	3828	1/1	0.96	0.18	43,43,43,43	0
58	MG	1A	3115	1/1	0.96	0.22	32,32,32,32	0
58	MG	1A	3574	1/1	0.96	0.16	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3450	1/1	0.96	0.20	48,48,48,48	0
58	MG	2A	3451	1/1	0.96	0.42	51,51,51,51	0
58	MG	1a	1659	1/1	0.96	0.13	40,40,40,40	0
58	MG	1A	3346	1/1	0.96	0.38	60,60,60,60	0
58	MG	1B	234	1/1	0.96	0.14	33,33,33,33	0
58	MG	2A	3456	1/1	0.96	0.39	44,44,44,44	0
58	MG	1A	3694	1/1	0.96	0.25	16,16,16,16	0
58	MG	2a	1707	1/1	0.96	0.16	51,51,51,51	0
58	MG	1A	3837	1/1	0.96	0.18	36,36,36,36	0
58	MG	2A	3008	1/1	0.96	0.29	46,46,46,46	0
58	MG	1A	3410	1/1	0.96	0.18	37,37,37,37	0
58	MG	2A	3461	1/1	0.96	0.34	45,45,45,45	0
58	MG	2A	3230	1/1	0.96	0.28	40,40,40,40	0
58	MG	1A	3696	1/1	0.96	0.15	28,28,28,28	0
58	MG	2A	3232	1/1	0.96	0.16	39,39,39,39	0
58	MG	2A	3465	1/1	0.96	0.22	58,58,58,58	0
58	MG	2a	1716	1/1	0.96	0.26	53,53,53,53	0
58	MG	1A	3577	1/1	0.96	0.23	35,35,35,35	0
58	MG	2A	3014	1/1	0.96	0.26	36,36,36,36	0
58	MG	1D	302	1/1	0.96	0.18	37,37,37,37	0
58	MG	1A	3846	1/1	0.96	0.16	27,27,27,27	0
58	MG	1A	3990	1/1	0.96	0.09	43,43,43,43	0
58	MG	2A	3758	1/1	0.96	0.18	47,47,47,47	0
58	MG	2A	3475	1/1	0.96	0.13	52,52,52,52	0
58	MG	2A	3476	1/1	0.96	0.19	38,38,38,38	0
58	MG	1A	3490	1/1	0.96	0.21	33,33,33,33	0
58	MG	2A	3479	1/1	0.96	0.12	38,38,38,38	0
58	MG	2A	3763	1/1	0.96	0.21	40,40,40,40	0
58	MG	2A	3019	1/1	0.96	0.23	34,34,34,34	0
58	MG	1A	3154	1/1	0.96	0.20	33,33,33,33	0
58	MG	2A	3766	1/1	0.96	0.19	51,51,51,51	0
58	MG	1A	3414	1/1	0.96	0.16	45,45,45,45	0
58	MG	2A	3023	1/1	0.96	0.13	49,49,49,49	0
58	MG	2a	1734	1/1	0.96	0.23	53,53,53,53	0
58	MG	1A	3994	1/1	0.96	0.22	21,21,21,21	0
58	MG	1A	3415	1/1	0.96	0.24	33,33,33,33	0
58	MG	2A	3772	1/1	0.96	0.10	46,46,46,46	0
58	MG	1A	3043	1/1	0.96	0.16	23,23,23,23	0
58	MG	2A	3249	1/1	0.96	0.20	58,58,58,58	0
58	MG	2A	3775	1/1	0.96	0.20	34,34,34,34	0
58	MG	2A	3028	1/1	0.96	0.17	45,45,45,45	0
58	MG	1E	303	1/1	0.96	0.34	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3030	1/1	0.96	0.19	37,37,37,37	0
58	MG	1E	305	1/1	0.96	0.18	17,17,17,17	0
58	MG	1A	3585	1/1	0.96	0.14	25,25,25,25	0
58	MG	1a	1683	1/1	0.96	0.08	55,55,55,55	0
58	MG	1A	3215	1/1	0.96	0.16	40,40,40,40	0
58	MG	1A	3855	1/1	0.96	0.14	52,52,52,52	0
58	MG	2A	3258	1/1	0.96	0.14	51,51,51,51	0
58	MG	1a	1687	1/1	0.96	0.25	58,58,58,58	0
58	MG	1A	3587	1/1	0.96	0.23	18,18,18,18	0
58	MG	2A	3040	1/1	0.96	0.25	40,40,40,40	0
58	MG	2a	1755	1/1	0.96	0.18	51,51,51,51	0
58	MG	1A	3044	1/1	0.96	0.15	28,28,28,28	0
58	MG	2A	3042	1/1	0.96	0.30	53,53,53,53	0
58	MG	2A	3043	1/1	0.96	0.16	61,61,61,61	0
58	MG	2A	3797	1/1	0.96	0.12	46,46,46,46	0
58	MG	1A	3355	1/1	0.96	0.26	46,46,46,46	0
58	MG	1A	3713	1/1	0.96	0.17	19,19,19,19	0
58	MG	1F	308	1/1	0.96	0.11	35,35,35,35	0
58	MG	1A	3047	1/1	0.96	0.19	25,25,25,25	0
58	MG	1A	3219	1/1	0.96	0.27	28,28,28,28	0
58	MG	1A	3359	1/1	0.96	0.20	48,48,48,48	0
58	MG	2A	3051	1/1	0.96	0.13	38,38,38,38	0
58	MG	2a	1770	1/1	0.96	0.17	48,48,48,48	0
58	MG	2A	3516	1/1	0.96	0.27	52,52,52,52	0
58	MG	1A	3426	1/1	0.96	0.15	37,37,37,37	0
58	MG	1A	3428	1/1	0.96	0.20	31,31,31,31	0
58	MG	1A	4013	1/1	0.96	0.09	43,43,43,43	0
58	MG	1a	1703	1/1	0.96	0.11	57,57,57,57	0
58	MG	2A	3522	1/1	0.96	0.25	37,37,37,37	0
58	MG	1a	1704	1/1	0.96	0.22	37,37,37,37	0
58	MG	1A	3429	1/1	0.96	0.18	34,34,34,34	0
58	MG	2A	3813	1/1	0.96	0.08	53,53,53,53	0
58	MG	2A	3814	1/1	0.96	0.21	43,43,43,43	0
58	MG	1A	4015	1/1	0.96	0.17	22,22,22,22	0
58	MG	2a	1783	1/1	0.96	0.22	60,60,60,60	0
58	MG	1I	201	1/1	0.96	0.10	35,35,35,35	0
58	MG	1A	3430	1/1	0.96	0.17	36,36,36,36	0
58	MG	1A	3138	1/1	0.96	0.15	18,18,18,18	0
58	MG	2A	3531	1/1	0.96	0.17	36,36,36,36	0
58	MG	2A	3822	1/1	0.96	0.19	29,29,29,29	0
58	MG	1A	3103	1/1	0.96	0.19	28,28,28,28	0
58	MG	1A	3509	1/1	0.96	0.09	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3433	1/1	0.96	0.18	36,36,36,36	0
58	MG	1A	3879	1/1	0.96	0.13	30,30,30,30	0
58	MG	2A	3830	1/1	0.96	0.21	53,53,53,53	0
58	MG	1A	4022	1/1	0.96	0.13	40,40,40,40	0
58	MG	1A	3143	1/1	0.96	0.25	9,9,9,9	0
58	MG	2A	3539	1/1	0.96	0.15	40,40,40,40	0
58	MG	2A	3835	1/1	0.96	0.13	57,57,57,57	0
58	MG	1P	202	1/1	0.96	0.14	24,24,24,24	0
58	MG	2a	1800	1/1	0.96	0.18	52,52,52,52	0
58	MG	1a	1719	1/1	0.96	0.24	33,33,33,33	0
58	MG	1A	3512	1/1	0.96	0.23	42,42,42,42	0
58	MG	1A	3105	1/1	0.96	0.12	35,35,35,35	0
58	MG	2A	3840	1/1	0.96	0.25	22,22,22,22	0
58	MG	1A	3049	1/1	0.96	0.20	15,15,15,15	0
58	MG	2A	3546	1/1	0.96	0.25	35,35,35,35	0
58	MG	1Q	206	1/1	0.96	0.19	41,41,41,41	0
58	MG	2a	1808	1/1	0.96	0.20	48,48,48,48	0
58	MG	1Q	207	1/1	0.96	0.36	36,36,36,36	0
58	MG	2a	1810	1/1	0.96	0.13	50,50,50,50	0
58	MG	1A	3515	1/1	0.96	0.13	15,15,15,15	0
58	MG	1A	3611	1/1	0.96	0.17	30,30,30,30	0
58	MG	1a	1727	1/1	0.96	0.22	47,47,47,47	0
58	MG	1A	3264	1/1	0.96	0.15	53,53,53,53	0
58	MG	1A	3613	1/1	0.96	0.17	33,33,33,33	0
58	MG	2A	3556	1/1	0.96	0.23	41,41,41,41	0
58	MG	1A	3891	1/1	0.96	0.13	28,28,28,28	0
58	MG	1A	3517	1/1	0.96	0.15	46,46,46,46	0
58	MG	1A	4034	1/1	0.96	0.19	32,32,32,32	0
58	MG	1A	3314	1/1	0.96	0.24	50,50,50,50	0
58	MG	1A	3369	1/1	0.96	0.25	32,32,32,32	0
58	MG	1A	3617	1/1	0.96	0.22	23,23,23,23	0
58	MG	1A	3370	1/1	0.96	0.10	31,31,31,31	0
58	MG	1A	3521	1/1	0.96	0.22	26,26,26,26	0
58	MG	2a	1830	1/1	0.96	0.13	50,50,50,50	0
58	MG	2A	3090	1/1	0.96	0.10	59,59,59,59	0
58	MG	1A	3522	1/1	0.96	0.21	23,23,23,23	0
58	MG	2A	3571	1/1	0.96	0.23	30,30,30,30	0
58	MG	1A	3523	1/1	0.96	0.13	21,21,21,21	0
58	MG	2A	3094	1/1	0.96	0.16	31,31,31,31	0
58	MG	2A	3095	1/1	0.96	0.34	37,37,37,37	0
58	MG	2A	3096	1/1	0.96	0.27	48,48,48,48	0
58	MG	2B	204	1/1	0.96	0.16	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2i	201	1/1	0.96	0.07	52,52,52,52	0
58	MG	1A	3901	1/1	0.96	0.15	46,46,46,46	0
58	MG	2A	3578	1/1	0.96	0.12	39,39,39,39	0
58	MG	2A	3321	1/1	0.96	0.20	45,45,45,45	0
58	MG	2B	209	1/1	0.96	0.12	49,49,49,49	0
58	MG	1A	3623	1/1	0.96	0.15	23,23,23,23	0
58	MG	1A	3754	1/1	0.96	0.20	25,25,25,25	0
58	MG	1A	3905	1/1	0.96	0.17	21,21,21,21	0
58	MG	1A	3003	1/1	0.96	0.32	26,26,26,26	0
58	MG	2A	3103	1/1	0.96	0.23	26,26,26,26	0
58	MG	1Y	202	1/1	0.96	0.20	55,55,55,55	0
58	MG	2A	3588	1/1	0.96	0.31	53,53,53,53	0
58	MG	1A	3907	1/1	0.96	0.20	16,16,16,16	0
58	MG	2B	219	1/1	0.96	0.19	71,71,71,71	0
58	MG	1A	3035	1/1	0.96	0.14	31,31,31,31	0
58	MG	1A	3196	1/1	0.96	0.18	24,24,24,24	0
58	MG	1A	3268	1/1	0.96	0.17	29,29,29,29	0
58	MG	1A	3912	1/1	0.96	0.23	28,28,28,28	0
58	MG	2A	3110	1/1	0.96	0.23	52,52,52,52	0
58	MG	1A	3450	1/1	0.96	0.21	31,31,31,31	0
58	MG	10	107	1/1	0.96	0.15	37,37,37,37	0
58	MG	2x	103	1/1	0.96	0.50	53,53,53,53	0
58	MG	2E	305	1/1	0.96	0.24	37,37,37,37	0
58	MG	1A	3322	1/1	0.96	0.18	43,43,43,43	0
58	MG	2A	3337	1/1	0.96	0.23	56,56,56,56	0
58	MG	1A	3230	1/1	0.96	0.23	25,25,25,25	0
58	MG	1A	3635	1/1	0.96	0.13	36,36,36,36	0
59	K	2x	101	1/1	0.96	0.18	43,43,43,43	0
58	MG	1A	3324	1/1	0.96	0.21	38,38,38,38	0
58	MG	2A	3602	1/1	0.96	0.13	41,41,41,41	0
58	MG	2F	305	1/1	0.96	0.16	33,33,33,33	0
58	MG	1A	3771	1/1	0.96	0.18	37,37,37,37	0
58	MG	2A	3376	1/1	0.97	0.18	42,42,42,42	0
58	MG	2A	3767	1/1	0.97	0.23	33,33,33,33	0
58	MG	2A	3209	1/1	0.97	0.19	37,37,37,37	0
58	MG	1A	3685	1/1	0.97	0.17	15,15,15,15	0
58	MG	1A	3161	1/1	0.97	0.21	28,28,28,28	0
58	MG	1A	3342	1/1	0.97	0.18	44,44,44,44	0
58	MG	1A	3023	1/1	0.97	0.18	10,10,10,10	0
58	MG	2a	1648	1/1	0.97	0.14	56,56,56,56	0
58	MG	1A	3792	1/1	0.97	0.18	34,34,34,34	0
58	MG	1A	3203	1/1	0.97	0.22	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3097	1/1	0.97	0.20	22,22,22,22	0
58	MG	2A	3776	1/1	0.97	0.11	55,55,55,55	0
58	MG	2A	3777	1/1	0.97	0.25	40,40,40,40	0
58	MG	2A	3579	1/1	0.97	0.17	48,48,48,48	0
58	MG	2A	3217	1/1	0.97	0.22	40,40,40,40	0
58	MG	1A	3076	1/1	0.97	0.25	15,15,15,15	0
58	MG	2A	3781	1/1	0.97	0.08	51,51,51,51	0
58	MG	2A	3219	1/1	0.97	0.25	32,32,32,32	0
58	MG	1A	3796	1/1	0.97	0.20	35,35,35,35	0
58	MG	1A	3296	1/1	0.97	0.24	53,53,53,53	0
58	MG	2A	3585	1/1	0.97	0.23	62,62,62,62	0
58	MG	1A	3348	1/1	0.97	0.15	25,25,25,25	0
58	MG	1A	3016	1/1	0.97	0.29	49,49,49,49	0
58	MG	1A	3050	1/1	0.97	0.33	34,34,34,34	0
58	MG	1A	3252	1/1	0.97	0.15	24,24,24,24	0
58	MG	1A	3081	1/1	0.97	0.27	28,28,28,28	0
58	MG	2A	3793	1/1	0.97	0.08	58,58,58,58	0
58	MG	2A	3227	1/1	0.97	0.47	54,54,54,54	0
58	MG	1A	4028	1/1	0.97	0.11	35,35,35,35	0
58	MG	1A	3104	1/1	0.97	0.24	26,26,26,26	0
58	MG	1A	3411	1/1	0.97	0.15	31,31,31,31	0
58	MG	1A	3172	1/1	0.97	0.26	8,8,8,8	0
58	MG	1A	3476	1/1	0.97	0.23	47,47,47,47	0
58	MG	2A	3234	1/1	0.97	0.20	37,37,37,37	0
58	MG	1A	3413	1/1	0.97	0.11	37,37,37,37	0
58	MG	1A	3926	1/1	0.97	0.14	22,22,22,22	0
58	MG	1A	3214	1/1	0.97	0.23	27,27,27,27	0
58	MG	1A	3708	1/1	0.97	0.09	28,28,28,28	0
58	MG	2A	3406	1/1	0.97	0.21	46,46,46,46	0
58	MG	1A	3257	1/1	0.97	0.18	21,21,21,21	0
58	MG	2a	1683	1/1	0.97	0.33	39,39,39,39	0
58	MG	1A	3711	1/1	0.97	0.23	38,38,38,38	0
58	MG	1A	3619	1/1	0.97	0.18	24,24,24,24	0
58	MG	1A	3545	1/1	0.97	0.25	21,21,21,21	0
58	MG	1A	3815	1/1	0.97	0.16	15,15,15,15	0
58	MG	1A	3038	1/1	0.97	0.16	16,16,16,16	0
58	MG	1E	310	1/1	0.97	0.21	16,16,16,16	0
58	MG	1A	3107	1/1	0.97	0.21	17,17,17,17	0
58	MG	1A	3482	1/1	0.97	0.23	30,30,30,30	0
58	MG	1a	1632	1/1	0.97	0.28	49,49,49,49	0
58	MG	1E	313	1/1	0.97	0.28	36,36,36,36	0
58	MG	1E	314	1/1	0.97	0.06	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3818	1/1	0.97	0.20	33,33,33,33	0
58	MG	2A	3615	1/1	0.97	0.20	50,50,50,50	0
58	MG	1A	3108	1/1	0.97	0.15	30,30,30,30	0
58	MG	1F	303	1/1	0.97	0.20	23,23,23,23	0
58	MG	1F	304	1/1	0.97	0.22	21,21,21,21	0
58	MG	1A	3721	1/1	0.97	0.14	29,29,29,29	0
58	MG	2A	3091	1/1	0.97	0.25	44,44,44,44	0
58	MG	2A	3826	1/1	0.97	0.12	49,49,49,49	0
58	MG	2A	3827	1/1	0.97	0.11	54,54,54,54	0
58	MG	2A	3828	1/1	0.97	0.20	51,51,51,51	0
58	MG	1A	3218	1/1	0.97	0.21	31,31,31,31	0
58	MG	1F	307	1/1	0.97	0.21	32,32,32,32	0
58	MG	1A	3723	1/1	0.97	0.19	40,40,40,40	0
58	MG	1A	3365	1/1	0.97	0.15	36,36,36,36	0
58	MG	2A	3261	1/1	0.97	0.19	42,42,42,42	0
58	MG	2A	3430	1/1	0.97	0.14	38,38,38,38	0
58	MG	1A	3827	1/1	0.97	0.26	16,16,16,16	0
58	MG	1A	3627	1/1	0.97	0.20	29,29,29,29	0
58	MG	2A	3630	1/1	0.97	0.16	33,33,33,33	0
58	MG	1A	3313	1/1	0.97	0.33	40,40,40,40	0
58	MG	1A	3367	1/1	0.97	0.18	27,27,27,27	0
58	MG	2a	1718	1/1	0.97	0.16	57,57,57,57	0
58	MG	1A	4055	1/1	0.97	0.15	36,36,36,36	0
58	MG	2A	3634	1/1	0.97	0.17	25,25,25,25	0
58	MG	1A	3425	1/1	0.97	0.14	33,33,33,33	0
58	MG	1A	3833	1/1	0.97	0.16	25,25,25,25	0
58	MG	1A	3733	1/1	0.97	0.20	19,19,19,19	0
58	MG	1A	3083	1/1	0.97	0.21	27,27,27,27	0
58	MG	1a	1654	1/1	0.97	0.24	46,46,46,46	0
58	MG	2A	3443	1/1	0.97	0.39	41,41,41,41	0
58	MG	1A	3634	1/1	0.97	0.17	21,21,21,21	0
58	MG	1N	203	1/1	0.97	0.27	27,27,27,27	0
58	MG	2A	3275	1/1	0.97	0.11	65,65,65,65	0
58	MG	1A	3840	1/1	0.97	0.12	43,43,43,43	0
58	MG	1A	3841	1/1	0.97	0.23	40,40,40,40	0
58	MG	1A	3427	1/1	0.97	0.24	51,51,51,51	0
58	MG	1O	202	1/1	0.97	0.19	47,47,47,47	0
58	MG	1A	3140	1/1	0.97	0.20	29,29,29,29	0
58	MG	2A	3859	1/1	0.97	0.05	62,62,62,62	0
58	MG	2a	1736	1/1	0.97	0.35	49,49,49,49	0
58	MG	1A	3142	1/1	0.97	0.17	20,20,20,20	0
58	MG	1A	4067	1/1	0.97	0.15	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3653	1/1	0.97	0.21	38,38,38,38	0
58	MG	2A	3863	1/1	0.97	0.28	44,44,44,44	0
58	MG	2A	3454	1/1	0.97	0.32	33,33,33,33	0
58	MG	2A	3865	1/1	0.97	0.11	64,64,64,64	0
58	MG	2A	3116	1/1	0.97	0.34	40,40,40,40	0
58	MG	2A	3867	1/1	0.97	0.12	38,38,38,38	0
58	MG	2A	3284	1/1	0.97	0.12	55,55,55,55	0
58	MG	2A	3657	1/1	0.97	0.27	46,46,46,46	0
58	MG	2B	201	1/1	0.97	0.28	60,60,60,60	0
58	MG	1a	1665	1/1	0.97	0.13	51,51,51,51	0
58	MG	1A	3561	1/1	0.97	0.12	15,15,15,15	0
58	MG	1A	3741	1/1	0.97	0.19	37,37,37,37	0
58	MG	1a	1668	1/1	0.97	0.25	51,51,51,51	0
58	MG	2a	1752	1/1	0.97	0.13	59,59,59,59	0
58	MG	1A	3562	1/1	0.97	0.19	29,29,29,29	0
58	MG	1A	3085	1/1	0.97	0.20	26,26,26,26	0
58	MG	2B	208	1/1	0.97	0.21	48,48,48,48	0
58	MG	1A	3320	1/1	0.97	0.16	22,22,22,22	0
58	MG	1A	3852	1/1	0.97	0.12	34,34,34,34	0
58	MG	1A	3008	1/1	0.97	0.29	15,15,15,15	0
58	MG	2a	1759	1/1	0.97	0.10	59,59,59,59	0
58	MG	1A	3087	1/1	0.97	0.17	22,22,22,22	0
58	MG	1A	4078	1/1	0.97	0.18	45,45,45,45	0
58	MG	2A	3469	1/1	0.97	0.10	46,46,46,46	0
58	MG	2a	1763	1/1	0.97	0.15	42,42,42,42	0
58	MG	2A	3671	1/1	0.97	0.15	50,50,50,50	0
58	MG	2A	3129	1/1	0.97	0.23	40,40,40,40	0
58	MG	1f	202	1/1	0.97	0.26	47,47,47,47	0
58	MG	1A	4079	1/1	0.97	0.20	45,45,45,45	0
58	MG	2D	301	1/1	0.97	0.14	31,31,31,31	0
58	MG	1A	3225	1/1	0.97	0.20	32,32,32,32	0
58	MG	1A	3435	1/1	0.97	0.13	40,40,40,40	0
58	MG	1A	3004	1/1	0.97	0.23	16,16,16,16	0
58	MG	2A	3478	1/1	0.97	0.12	51,51,51,51	0
58	MG	1a	1680	1/1	0.97	0.10	60,60,60,60	0
58	MG	1U	202	1/1	0.97	0.22	31,31,31,31	0
58	MG	2E	302	1/1	0.97	0.15	45,45,45,45	0
58	MG	2A	3137	1/1	0.97	0.23	31,31,31,31	0
58	MG	2E	304	1/1	0.97	0.20	32,32,32,32	0
58	MG	1t	201	1/1	0.97	0.12	46,46,46,46	0
58	MG	1U	203	1/1	0.97	0.14	26,26,26,26	0
58	MG	2A	3140	1/1	0.97	0.32	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2E	308	1/1	0.97	0.31	32,32,32,32	0
58	MG	2A	3489	1/1	0.97	0.17	55,55,55,55	0
58	MG	1w	101	1/1	0.97	0.20	35,35,35,35	0
58	MG	1w	102	1/1	0.97	0.44	67,67,67,67	0
58	MG	1A	3968	1/1	0.97	0.19	43,43,43,43	0
58	MG	2A	3312	1/1	0.97	0.16	55,55,55,55	0
58	MG	1U	211	1/1	0.97	0.16	28,28,28,28	0
58	MG	1V	203	1/1	0.97	0.23	39,39,39,39	0
58	MG	1A	3014	1/1	0.97	0.18	18,18,18,18	0
58	MG	1A	3860	1/1	0.97	0.06	49,49,49,49	0
58	MG	1a	1689	1/1	0.97	0.32	30,30,30,30	0
58	MG	1a	1690	1/1	0.97	0.24	55,55,55,55	0
58	MG	1A	3188	1/1	0.97	0.14	40,40,40,40	0
58	MG	2A	3699	1/1	0.97	0.14	50,50,50,50	0
58	MG	2A	3152	1/1	0.97	0.18	54,54,54,54	0
58	MG	1A	4090	1/1	0.97	0.28	50,50,50,50	0
58	MG	1A	3090	1/1	0.97	0.25	28,28,28,28	0
58	MG	1A	3067	1/1	0.97	0.25	23,23,23,23	0
58	MG	1A	3441	1/1	0.97	0.29	39,39,39,39	0
58	MG	1A	3234	1/1	0.97	0.13	33,33,33,33	0
58	MG	1A	3867	1/1	0.97	0.17	23,23,23,23	0
58	MG	1A	3868	1/1	0.97	0.22	19,19,19,19	0
58	MG	1A	3757	1/1	0.97	0.26	47,47,47,47	0
58	MG	1x	111	1/1	0.97	0.10	56,56,56,56	0
58	MG	1x	112	1/1	0.97	0.27	52,52,52,52	0
58	MG	1a	1701	1/1	0.97	0.09	44,44,44,44	0
58	MG	1A	3118	1/1	0.97	0.19	19,19,19,19	0
58	MG	1A	3279	1/1	0.97	0.18	23,23,23,23	0
58	MG	1A	3983	1/1	0.97	0.10	54,54,54,54	0
58	MG	1A	3761	1/1	0.97	0.20	33,33,33,33	0
58	MG	23	101	1/1	0.97	0.26	51,51,51,51	0
58	MG	23	102	1/1	0.97	0.21	40,40,40,40	0
58	MG	1A	3445	1/1	0.97	0.21	31,31,31,31	0
58	MG	10	102	1/1	0.97	0.23	44,44,44,44	0
58	MG	10	103	1/1	0.97	0.10	30,30,30,30	0
58	MG	10	104	1/1	0.97	0.24	45,45,45,45	0
58	MG	2a	1821	1/1	0.97	0.24	71,71,71,71	0
58	MG	1a	1710	1/1	0.97	0.14	41,41,41,41	0
58	MG	2a	1823	1/1	0.97	0.30	39,39,39,39	0
58	MG	1A	3446	1/1	0.97	0.14	48,48,48,48	0
58	MG	2a	1825	1/1	0.97	0.10	44,44,44,44	0
58	MG	1A	3581	1/1	0.97	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
58	MG	1A	3447	1/1	0.97	0.17	41,41,41,41	0
58	MG	1A	3583	1/1	0.97	0.12	40,40,40,40	0
58	MG	11	102	1/1	0.97	0.20	36,36,36,36	0
58	MG	1A	3015	1/1	0.97	0.11	26,26,26,26	0
58	MG	2A	3730	1/1	0.97	0.10	39,39,39,39	0
58	MG	2a	1602	1/1	0.97	0.28	51,51,51,51	0
58	MG	2a	1835	1/1	0.97	0.22	52,52,52,52	0
58	MG	2A	3347	1/1	0.97	0.12	58,58,58,58	0
58	MG	1A	3120	1/1	0.97	0.30	38,38,38,38	0
58	MG	2A	3020	1/1	0.97	0.15	55,55,55,55	0
58	MG	1A	3669	1/1	0.97	0.21	19,19,19,19	0
58	MG	1A	3058	1/1	0.97	0.17	13,13,13,13	0
58	MG	2A	3736	1/1	0.97	0.13	44,44,44,44	0
58	MG	1A	3195	1/1	0.97	0.19	25,25,25,25	0
58	MG	1B	203	1/1	0.97	0.20	38,38,38,38	0
58	MG	1A	3673	1/1	0.97	0.14	16,16,16,16	0
58	MG	2A	3026	1/1	0.97	0.11	40,40,40,40	0
58	MG	13	102	1/1	0.97	0.21	25,25,25,25	0
58	MG	13	103	1/1	0.97	0.28	34,34,34,34	0
58	MG	1A	3453	1/1	0.97	0.20	25,25,25,25	0
58	MG	2A	3545	1/1	0.97	0.22	33,33,33,33	0
58	MG	2q	201	1/1	0.97	0.10	63,63,63,63	0
58	MG	13	105	1/1	0.97	0.18	37,37,37,37	0
58	MG	2A	3031	1/1	0.97	0.14	51,51,51,51	0
58	MG	2A	3548	1/1	0.97	0.18	40,40,40,40	0
58	MG	1B	206	1/1	0.97	0.10	39,39,39,39	0
58	MG	1A	3997	1/1	0.97	0.19	20,20,20,20	0
58	MG	1A	3072	1/1	0.97	0.20	20,20,20,20	0
58	MG	2A	3552	1/1	0.97	0.27	40,40,40,40	0
58	MG	1A	3892	1/1	0.97	0.10	48,48,48,48	0
58	MG	2a	1625	1/1	0.97	0.16	56,56,56,56	0
58	MG	1A	3676	1/1	0.97	0.15	33,33,33,33	0
58	MG	1A	3392	1/1	0.97	0.21	22,22,22,22	0
58	MG	1A	3780	1/1	0.97	0.21	22,22,22,22	0
58	MG	1a	1735	1/1	0.97	0.12	42,42,42,42	0
58	MG	2A	3558	1/1	0.97	0.23	35,35,35,35	0
58	MG	2a	1631	1/1	0.97	0.26	44,44,44,44	0
58	MG	1A	3287	1/1	0.97	0.16	34,34,34,34	0
58	MG	1A	3679	1/1	0.97	0.14	21,21,21,21	0
58	MG	2a	1634	1/1	0.97	0.10	57,57,57,57	0
58	MG	1A	3288	1/1	0.97	0.16	27,27,27,27	0
58	MG	1A	3593	1/1	0.97	0.19	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	ZN	1n	103	1/1	0.97	0.10	53,53,53,53	0
58	MG	1A	3159	1/1	0.97	0.20	29,29,29,29	0
58	MG	1A	3073	1/1	0.97	0.17	9,9,9,9	0
60	ZN	29	501	1/1	0.97	0.08	55,55,55,55	0
58	MG	1A	3684	1/1	0.97	0.18	16,16,16,16	0
61	SF4	2d	303	8/8	0.97	0.09	56,63,69,75	0
58	MG	2a	1694	1/1	0.98	0.20	39,39,39,39	0
58	MG	1A	3902	1/1	0.98	0.11	33,33,33,33	0
58	MG	2A	3083	1/1	0.98	0.20	43,43,43,43	0
58	MG	1A	3729	1/1	0.98	0.16	25,25,25,25	0
58	MG	1A	3075	1/1	0.98	0.16	22,22,22,22	0
58	MG	2A	3697	1/1	0.98	0.30	28,28,28,28	0
58	MG	2a	1700	1/1	0.98	0.31	34,34,34,34	0
58	MG	1a	1661	1/1	0.98	0.14	58,58,58,58	0
58	MG	1A	3212	1/1	0.98	0.17	23,23,23,23	0
58	MG	1A	3732	1/1	0.98	0.24	33,33,33,33	0
58	MG	2A	3701	1/1	0.98	0.20	35,35,35,35	0
58	MG	1A	3656	1/1	0.98	0.22	15,15,15,15	0
58	MG	1A	3908	1/1	0.98	0.23	56,56,56,56	0
58	MG	2A	3233	1/1	0.98	0.26	44,44,44,44	0
58	MG	1U	205	1/1	0.98	0.15	29,29,29,29	0
58	MG	1U	206	1/1	0.98	0.18	20,20,20,20	0
58	MG	1U	209	1/1	0.98	0.16	25,25,25,25	0
58	MG	2A	3708	1/1	0.98	0.15	29,29,29,29	0
58	MG	1U	210	1/1	0.98	0.15	26,26,26,26	0
58	MG	1A	3657	1/1	0.98	0.21	22,22,22,22	0
58	MG	1V	202	1/1	0.98	0.17	21,21,21,21	0
58	MG	1A	3658	1/1	0.98	0.24	15,15,15,15	0
58	MG	1V	204	1/1	0.98	0.14	27,27,27,27	0
58	MG	2A	3099	1/1	0.98	0.09	34,34,34,34	0
58	MG	1A	3028	1/1	0.98	0.14	28,28,28,28	0
58	MG	2A	3244	1/1	0.98	0.31	43,43,43,43	0
58	MG	1A	3535	1/1	0.98	0.21	33,33,33,33	0
58	MG	1A	4007	1/1	0.98	0.17	13,13,13,13	0
58	MG	2D	304	1/1	0.98	0.21	31,31,31,31	0
58	MG	1A	4008	1/1	0.98	0.18	16,16,16,16	0
58	MG	1A	3051	1/1	0.98	0.19	15,15,15,15	0
58	MG	1A	4010	1/1	0.98	0.09	28,28,28,28	0
58	MG	1A	3128	1/1	0.98	0.15	33,33,33,33	0
58	MG	1X	103	1/1	0.98	0.23	30,30,30,30	0
58	MG	1A	3383	1/1	0.98	0.15	28,28,28,28	0
58	MG	1A	3916	1/1	0.98	0.18	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3726	1/1	0.98	0.25	40,40,40,40	0
58	MG	1A	3152	1/1	0.98	0.21	26,26,26,26	0
58	MG	1a	1685	1/1	0.98	0.19	46,46,46,46	0
58	MG	1A	3385	1/1	0.98	0.18	36,36,36,36	0
58	MG	1A	3110	1/1	0.98	0.17	23,23,23,23	0
58	MG	1Y	203	1/1	0.98	0.14	31,31,31,31	0
58	MG	1A	3042	1/1	0.98	0.14	21,21,21,21	0
58	MG	1A	3826	1/1	0.98	0.13	61,61,61,61	0
58	MG	1A	3012	1/1	0.98	0.14	24,24,24,24	0
58	MG	2A	3567	1/1	0.98	0.25	53,53,53,53	0
58	MG	1A	3156	1/1	0.98	0.31	33,33,33,33	0
58	MG	1A	3829	1/1	0.98	0.11	22,22,22,22	0
58	MG	1A	3298	1/1	0.98	0.16	35,35,35,35	0
58	MG	2A	3121	1/1	0.98	0.17	59,59,59,59	0
58	MG	1A	3604	1/1	0.98	0.20	25,25,25,25	0
58	MG	2A	3267	1/1	0.98	0.22	46,46,46,46	0
58	MG	1A	3672	1/1	0.98	0.20	13,13,13,13	0
58	MG	2A	3576	1/1	0.98	0.14	53,53,53,53	0
58	MG	1A	3605	1/1	0.98	0.31	53,53,53,53	0
58	MG	1A	3834	1/1	0.98	0.16	21,21,21,21	0
58	MG	1A	3299	1/1	0.98	0.20	34,34,34,34	0
58	MG	1a	1700	1/1	0.98	0.29	52,52,52,52	0
58	MG	1B	224	1/1	0.98	0.21	34,34,34,34	0
58	MG	1A	3030	1/1	0.98	0.17	24,24,24,24	0
58	MG	1A	3838	1/1	0.98	0.16	28,28,28,28	0
58	MG	1A	3045	1/1	0.98	0.17	29,29,29,29	0
58	MG	1A	3134	1/1	0.98	0.17	25,25,25,25	0
58	MG	1A	3610	1/1	0.98	0.18	34,34,34,34	0
58	MG	1A	3496	1/1	0.98	0.22	25,25,25,25	0
58	MG	1A	3843	1/1	0.98	0.20	46,46,46,46	0
58	MG	1A	3303	1/1	0.98	0.36	22,22,22,22	0
58	MG	2A	3427	1/1	0.98	0.25	43,43,43,43	0
58	MG	1A	3760	1/1	0.98	0.15	28,28,28,28	0
58	MG	1A	3135	1/1	0.98	0.18	33,33,33,33	0
58	MG	1A	3349	1/1	0.98	0.19	25,25,25,25	0
58	MG	1A	3763	1/1	0.98	0.15	27,27,27,27	0
58	MG	1A	3162	1/1	0.98	0.18	19,19,19,19	0
58	MG	1A	3765	1/1	0.98	0.16	17,17,17,17	0
58	MG	25	103	1/1	0.98	0.19	57,57,57,57	0
58	MG	2a	1769	1/1	0.98	0.12	42,42,42,42	0
58	MG	1A	3352	1/1	0.98	0.15	30,30,30,30	0
58	MG	1A	3098	1/1	0.98	0.26	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1D	304	1/1	0.98	0.28	36,36,36,36	0
58	MG	27	101	1/1	0.98	0.36	40,40,40,40	0
58	MG	2A	3437	1/1	0.98	0.13	51,51,51,51	0
58	MG	1A	3768	1/1	0.98	0.15	41,41,41,41	0
58	MG	1A	3503	1/1	0.98	0.22	21,21,21,21	0
58	MG	1A	3687	1/1	0.98	0.15	23,23,23,23	0
58	MG	1A	3857	1/1	0.98	0.21	36,36,36,36	0
58	MG	2A	3442	1/1	0.98	0.24	42,42,42,42	0
58	MG	2a	1780	1/1	0.98	0.18	45,45,45,45	0
58	MG	2A	3150	1/1	0.98	0.24	34,34,34,34	0
58	MG	2A	3010	1/1	0.98	0.36	54,54,54,54	0
58	MG	1A	3558	1/1	0.98	0.19	18,18,18,18	0
58	MG	1A	3227	1/1	0.98	0.24	32,32,32,32	0
58	MG	2A	3013	1/1	0.98	0.11	32,32,32,32	0
58	MG	17	104	1/1	0.98	0.15	44,44,44,44	0
58	MG	1A	3451	1/1	0.98	0.14	26,26,26,26	0
58	MG	1A	4051	1/1	0.98	0.19	26,26,26,26	0
58	MG	1A	3046	1/1	0.98	0.24	17,17,17,17	0
58	MG	1E	304	1/1	0.98	0.16	20,20,20,20	0
58	MG	2A	3161	1/1	0.98	0.17	37,37,37,37	0
58	MG	1A	3039	1/1	0.98	0.29	28,28,28,28	0
58	MG	19	101	1/1	0.98	0.18	39,39,39,39	0
58	MG	1A	3863	1/1	0.98	0.23	14,14,14,14	0
58	MG	2a	1795	1/1	0.98	0.16	41,41,41,41	0
58	MG	1E	307	1/1	0.98	0.15	29,29,29,29	0
58	MG	1E	308	1/1	0.98	0.16	26,26,26,26	0
58	MG	2A	3622	1/1	0.98	0.09	39,39,39,39	0
58	MG	2A	3792	1/1	0.98	0.07	53,53,53,53	0
58	MG	1A	3101	1/1	0.98	0.18	38,38,38,38	0
58	MG	1A	3231	1/1	0.98	0.19	19,19,19,19	0
58	MG	1A	3232	1/1	0.98	0.19	21,21,21,21	0
58	MG	1A	3269	1/1	0.98	0.15	46,46,46,46	0
58	MG	1A	3628	1/1	0.98	0.24	10,10,10,10	0
58	MG	1A	3141	1/1	0.98	0.20	37,37,37,37	0
58	MG	1F	301	1/1	0.98	0.17	26,26,26,26	0
58	MG	1a	1611	1/1	0.98	0.31	18,18,18,18	0
58	MG	2A	3467	1/1	0.98	0.12	47,47,47,47	0
58	MG	1A	3409	1/1	0.98	0.30	34,34,34,34	0
58	MG	1A	3070	1/1	0.98	0.26	11,11,11,11	0
58	MG	2A	3470	1/1	0.98	0.32	22,22,22,22	0
58	MG	1A	3632	1/1	0.98	0.27	29,29,29,29	0
58	MG	1A	3874	1/1	0.98	0.21	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3473	1/1	0.98	0.20	52,52,52,52	0
58	MG	1A	3200	1/1	0.98	0.14	21,21,21,21	0
58	MG	1A	3048	1/1	0.98	0.20	33,33,33,33	0
58	MG	2A	3641	1/1	0.98	0.15	38,38,38,38	0
58	MG	2A	3038	1/1	0.98	0.25	14,14,14,14	0
58	MG	2a	1639	1/1	0.98	0.34	48,48,48,48	0
58	MG	1A	3706	1/1	0.98	0.20	35,35,35,35	0
58	MG	1a	1752	1/1	0.98	0.21	48,48,48,48	0
58	MG	1F	309	1/1	0.98	0.18	22,22,22,22	0
58	MG	1A	3878	1/1	0.98	0.18	20,20,20,20	0
58	MG	1A	3202	1/1	0.98	0.19	23,23,23,23	0
58	MG	2a	1826	1/1	0.98	0.15	58,58,58,58	0
58	MG	2A	3482	1/1	0.98	0.13	43,43,43,43	0
58	MG	1A	3031	1/1	0.98	0.20	22,22,22,22	0
58	MG	1A	3204	1/1	0.98	0.18	27,27,27,27	0
58	MG	2A	3485	1/1	0.98	0.18	43,43,43,43	0
58	MG	2A	3821	1/1	0.98	0.19	40,40,40,40	0
58	MG	2a	1832	1/1	0.98	0.15	56,56,56,56	0
58	MG	1G	201	1/1	0.98	0.16	32,32,32,32	0
58	MG	2A	3488	1/1	0.98	0.28	51,51,51,51	0
58	MG	1A	4073	1/1	0.98	0.26	9,9,9,9	0
58	MG	1A	3466	1/1	0.98	0.23	50,50,50,50	0
58	MG	2A	3049	1/1	0.98	0.32	18,18,18,18	0
58	MG	2e	201	1/1	0.98	0.14	47,47,47,47	0
58	MG	1A	3278	1/1	0.98	0.09	40,40,40,40	0
58	MG	1A	3977	1/1	0.98	0.20	41,41,41,41	0
58	MG	1H	201	1/1	0.98	0.37	40,40,40,40	0
58	MG	1A	3240	1/1	0.98	0.19	21,21,21,21	0
58	MG	1A	3061	1/1	0.98	0.22	24,24,24,24	0
58	MG	1A	4080	1/1	0.98	0.18	30,30,30,30	0
58	MG	2A	3833	1/1	0.98	0.24	25,25,25,25	0
58	MG	1A	3886	1/1	0.98	0.17	22,22,22,22	0
58	MG	2a	1663	1/1	0.98	0.14	66,66,66,66	0
58	MG	1A	3887	1/1	0.98	0.16	16,16,16,16	0
58	MG	1A	3982	1/1	0.98	0.08	49,49,49,49	0
58	MG	1A	3716	1/1	0.98	0.22	22,22,22,22	0
58	MG	1A	3242	1/1	0.98	0.20	15,15,15,15	0
58	MG	2a	1668	1/1	0.98	0.15	58,58,58,58	0
58	MG	1A	4086	1/1	0.98	0.25	23,23,23,23	0
58	MG	1A	3718	1/1	0.98	0.22	34,34,34,34	0
58	MG	1A	3106	1/1	0.98	0.20	32,32,32,32	0
58	MG	1P	201	1/1	0.98	0.18	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3644	1/1	0.98	0.13	18,18,18,18	0
58	MG	2A	3674	1/1	0.98	0.19	32,32,32,32	0
58	MG	1P	203	1/1	0.98	0.20	23,23,23,23	0
58	MG	1a	1644	1/1	0.98	0.18	51,51,51,51	0
58	MG	1P	204	1/1	0.98	0.20	34,34,34,34	0
58	MG	1A	3421	1/1	0.98	0.16	31,31,31,31	0
58	MG	1Q	203	1/1	0.98	0.27	25,25,25,25	0
58	MG	1a	1648	1/1	0.98	0.24	40,40,40,40	0
58	MG	2A	3514	1/1	0.98	0.17	51,51,51,51	0
58	MG	1A	3801	1/1	0.98	0.15	17,17,17,17	0
58	MG	2A	3853	1/1	0.98	0.13	55,55,55,55	0
58	MG	1A	3422	1/1	0.98	0.31	36,36,36,36	0
58	MG	1A	3374	1/1	0.98	0.29	41,41,41,41	0
59	K	1A	3569	1/1	0.98	0.18	37,37,37,37	0
58	MG	1A	3175	1/1	0.98	0.15	19,19,19,19	0
58	MG	1A	3147	1/1	0.98	0.23	16,16,16,16	0
58	MG	2A	3520	1/1	0.98	0.24	16,16,16,16	0
58	MG	1R	201	1/1	0.98	0.15	36,36,36,36	0
58	MG	1R	202	1/1	0.98	0.14	26,26,26,26	0
60	ZN	25	107	1/1	0.98	0.16	51,51,51,51	0
58	MG	1A	3177	1/1	0.98	0.20	23,23,23,23	0
58	MG	1A	3728	1/1	0.98	0.10	21,21,21,21	0
58	MG	2A	3525	1/1	0.98	0.16	46,46,46,46	0
58	MG	1W	204	1/1	0.99	0.20	28,28,28,28	0
58	MG	1A	3178	1/1	0.99	0.20	22,22,22,22	0
58	MG	1A	3844	1/1	0.99	0.13	42,42,42,42	0
58	MG	1A	3033	1/1	0.99	0.17	25,25,25,25	0
58	MG	1A	3280	1/1	0.99	0.19	19,19,19,19	0
58	MG	2A	3667	1/1	0.99	0.23	48,48,48,48	0
58	MG	1A	3180	1/1	0.99	0.17	16,16,16,16	0
58	MG	2A	3746	1/1	0.99	0.19	31,31,31,31	0
58	MG	1A	3358	1/1	0.99	0.17	24,24,24,24	0
58	MG	1A	3653	1/1	0.99	0.20	10,10,10,10	0
58	MG	1A	3942	1/1	0.99	0.20	9,9,9,9	0
58	MG	1A	3726	1/1	0.99	0.17	9,9,9,9	0
58	MG	1A	3084	1/1	0.99	0.21	24,24,24,24	0
58	MG	1a	1750	1/1	0.99	0.19	36,36,36,36	0
58	MG	1A	4088	1/1	0.99	0.22	26,26,26,26	0
58	MG	1A	3689	1/1	0.99	0.23	21,21,21,21	0
58	MG	1A	3163	1/1	0.99	0.17	18,18,18,18	0
58	MG	1A	3560	1/1	0.99	0.12	24,24,24,24	0
58	MG	2a	1815	1/1	0.99	0.18	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3284	1/1	0.99	0.17	27,27,27,27	0
58	MG	1A	3308	1/1	0.99	0.23	16,16,16,16	0
58	MG	2A	3529	1/1	0.99	0.24	37,37,37,37	0
58	MG	1A	3164	1/1	0.99	0.16	23,23,23,23	0
58	MG	1A	3034	1/1	0.99	0.20	23,23,23,23	0
58	MG	1A	3010	1/1	0.99	0.20	17,17,17,17	0
58	MG	1A	3816	1/1	0.99	0.24	11,11,11,11	0
58	MG	1D	303	1/1	0.99	0.27	16,16,16,16	0
58	MG	1A	3136	1/1	0.99	0.21	29,29,29,29	0
58	MG	1A	3737	1/1	0.99	0.17	41,41,41,41	0
58	MG	2X	102	1/1	0.99	0.15	32,32,32,32	0
58	MG	1Q	201	1/1	0.99	0.20	29,29,29,29	0
58	MG	2A	3538	1/1	0.99	0.19	27,27,27,27	0
58	MG	1A	3819	1/1	0.99	0.24	17,17,17,17	0
58	MG	1A	3206	1/1	0.99	0.28	16,16,16,16	0
58	MG	1w	106	1/1	0.99	0.25	43,43,43,43	0
58	MG	1A	3699	1/1	0.99	0.16	19,19,19,19	0
58	MG	1A	3036	1/1	0.99	0.20	22,22,22,22	0
58	MG	1A	3315	1/1	0.99	0.23	49,49,49,49	0
58	MG	2A	3854	1/1	0.99	0.16	45,45,45,45	0
58	MG	1A	3021	1/1	0.99	0.19	11,11,11,11	0
58	MG	1A	3602	1/1	0.99	0.13	20,20,20,20	0
58	MG	1A	3483	1/1	0.99	0.19	36,36,36,36	0
58	MG	1A	3871	1/1	0.99	0.16	27,27,27,27	0
58	MG	1A	3125	1/1	0.99	0.19	25,25,25,25	0
58	MG	1S	201	1/1	0.99	0.13	35,35,35,35	0
58	MG	15	102	1/1	0.99	0.14	30,30,30,30	0
58	MG	1A	4060	1/1	0.99	0.22	9,9,9,9	0
58	MG	1A	3318	1/1	0.99	0.27	39,39,39,39	0
58	MG	1A	3052	1/1	0.99	0.26	17,17,17,17	0
58	MG	1A	3078	1/1	0.99	0.16	22,22,22,22	0
58	MG	1a	1715	1/1	0.99	0.28	37,37,37,37	0
58	MG	1A	3079	1/1	0.99	0.19	27,27,27,27	0
58	MG	1U	201	1/1	0.99	0.16	15,15,15,15	0
58	MG	2A	3486	1/1	0.99	0.28	22,22,22,22	0
58	MG	2A	3790	1/1	0.99	0.13	52,52,52,52	0
58	MG	2A	3560	1/1	0.99	0.15	55,55,55,55	0
58	MG	1A	3710	1/1	0.99	0.22	22,22,22,22	0
58	MG	1A	3022	1/1	0.99	0.15	33,33,33,33	0
58	MG	17	102	1/1	0.99	0.12	23,23,23,23	0
58	MG	2A	3639	1/1	0.99	0.24	34,34,34,34	0
58	MG	1A	3158	1/1	0.99	0.26	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3835	1/1	0.99	0.17	23,23,23,23	0
58	MG	1A	3275	1/1	0.99	0.18	17,17,17,17	0
58	MG	1U	207	1/1	0.99	0.22	25,25,25,25	0
58	MG	2A	3568	1/1	0.99	0.18	39,39,39,39	0
58	MG	1U	208	1/1	0.99	0.16	25,25,25,25	0
58	MG	2A	3078	1/1	0.99	0.26	20,20,20,20	0
58	MG	18	103	1/1	0.99	0.17	30,30,30,30	0
58	MG	1A	3351	1/1	0.99	0.14	29,29,29,29	0
58	MG	2A	3287	1/1	0.99	0.15	48,48,48,48	0
58	MG	1A	3032	1/1	0.99	0.22	18,18,18,18	0
58	MG	2B	218	1/1	0.99	0.15	56,56,56,56	0
58	MG	1A	3756	1/1	0.99	0.21	11,11,11,11	0
58	MG	1V	201	1/1	0.99	0.16	19,19,19,19	0
58	MG	1B	214	1/1	0.99	0.31	48,48,48,48	0
60	ZN	1Y	204	1/1	0.99	0.10	54,54,54,54	0
58	MG	1A	3071	1/1	0.99	0.29	9,9,9,9	0
60	ZN	15	108	1/1	0.99	0.14	35,35,35,35	0
60	ZN	16	103	1/1	0.99	0.16	35,35,35,35	0
60	ZN	19	102	1/1	0.99	0.14	38,38,38,38	0
58	MG	1A	3646	1/1	0.99	0.15	25,25,25,25	0
58	MG	1A	3647	1/1	0.99	0.14	15,15,15,15	0
58	MG	2A	3156	1/1	0.99	0.24	26,26,26,26	0
58	MG	1A	3888	1/1	0.99	0.19	28,28,28,28	0
60	ZN	26	501	1/1	0.99	0.11	50,50,50,50	0
58	MG	1F	310	1/1	0.99	0.16	21,21,21,21	0
58	MG	1A	4077	1/1	0.99	0.17	15,15,15,15	0
61	SF4	1d	302	8/8	0.99	0.08	48,53,54,65	0
58	MG	1B	220	1/1	0.99	0.28	33,33,33,33	0
58	MG	1A	3714	1/1	1.00	0.18	10,10,10,10	0

6.5 Other polymers (i)

There are no such residues in this entry.