



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 7, 2022 – 07:37 PM EDT

PDB ID : 7U2H
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with mRNA, aminoacylated A-site Gly-NH-tRNA_{gly}, aminoacylated P-site fMet-NH-tRNA_{met}, and deacylated E-site tRNA_{gly} at 2.55Å resolution
Authors : Syroegin, E.A.; Aleksandrova, E.V.; Polikanov, Y.S.
Deposited on : 2022-02-24
Resolution : 2.55 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at <http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
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)	:	2.29

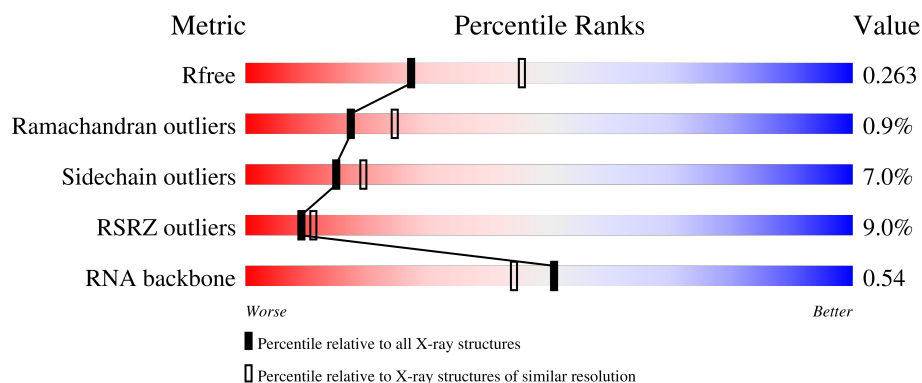
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1284 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)
RNA backbone	3102	1026 (2.88-2.20)

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

Mol	Chain	Length	Quality of chain
1	1A	2915	<div> <div>3%</div> <div>82%</div> <div>15%</div> <div>..</div> </div>
1	2A	2915	<div> <div>4%</div> <div>80%</div> <div>16%</div> <div>.</div> </div>
2	1B	121	<div> <div>93%</div> <div>7%</div> <div>.</div> </div>
2	2B	121	<div> <div>2%</div> <div>79%</div> <div>21%</div> <div>.</div> </div>
3	1D	276	<div> <div>%</div> <div>95%</div> <div>.</div> </div>

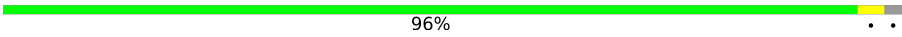
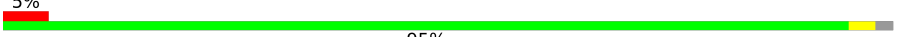
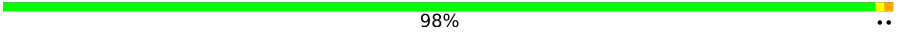
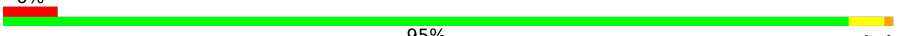
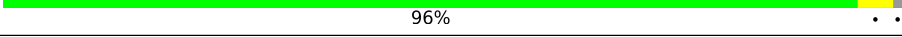
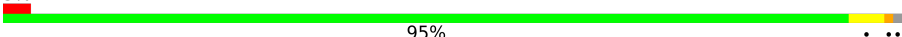

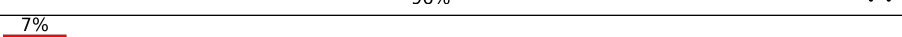
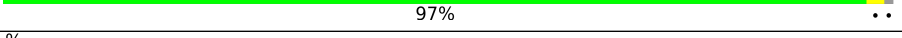


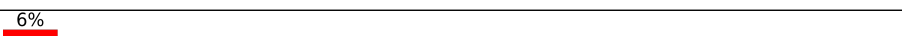
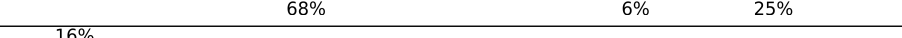

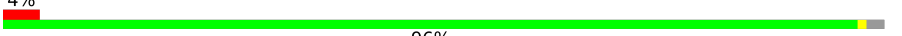

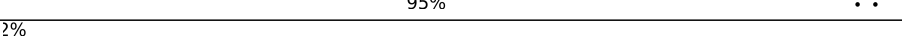
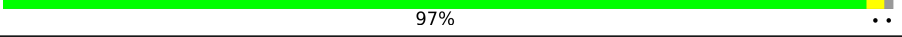


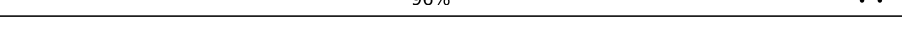
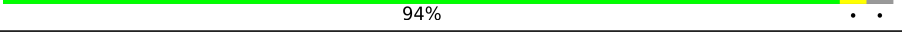



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Mol	Chain	Length	Quality of chain
3	2D	276	
4	1E	206	
4	2E	206	
5	1F	210	
5	2F	210	
6	1G	182	
6	2G	182	
7	1H	180	
7	2H	180	
8	1I	148	
8	2I	148	
9	1N	140	
9	2N	140	
10	1O	122	
10	2O	122	
11	1P	150	
11	2P	150	
12	1Q	141	
12	2Q	141	
13	1R	118	
13	2R	118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

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Mol	Chain	Length	Quality of chain
16	1U	118	 96% ..
16	2U	118	 5% 95% ..
17	1V	101	 98% ..
17	2V	101	 6% 95% ..
18	1W	113	 96% ..
18	2W	113	 3% 95% ..
19	1X	96	 2% 96% ..
19	2X	96	 7% 97% ..
20	1Y	110	 % 93% 5% ..
20	2Y	110	 11% 88% 9% .
21	1Z	206	 6% 68% 6% 25%
21	2Z	206	 16% 70% 7% 22%
22	10	85	 4% 96% ..
22	20	85	 21% 95% ..
23	11	98	 2% 97% ..
23	21	98	 8% 92% 7% .
24	12	72	 96% ..
24	22	72	 94% ..
25	13	60	 90% 8% .
25	23	60	 17% 95% ...
26	14	71	 7% 80% 15% ..
26	24	71	 42% 76% 20% ..
27	15	60	 2% 95% ..
27	25	60	 92% 7% .
28	16	54	 94% ..

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

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Mol	Chain	Length	Quality of chain
41	1j	105	
41	2j	105	
42	1k	129	
42	2k	129	
43	1l	132	
43	2l	132	
44	1m	126	
44	2m	126	
45	1n	61	
45	2n	61	
46	1o	89	
46	2o	89	
47	1p	88	
47	2p	88	
48	1q	105	
48	2q	105	
49	1r	88	
49	2r	88	
50	1s	93	
50	2s	93	
51	1t	106	
51	2t	106	
52	1u	27	
52	2u	27	
53	1v	24	

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Mol	Chain	Length	Quality of chain
53	2v	24	
54	1w	74	
54	2w	74	
55	1x	77	
55	2x	77	
56	1y	74	
56	2y	74	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	PSU	1w	55	-	-	-	X
56	5MU	1y	54	-	-	-	X
56	PSU	1y	55	-	-	-	X
56	5MU	2y	54	-	-	-	X
56	PSU	2y	55	-	-	-	X
57	MG	1A	3346	-	-	-	X
57	MG	1a	1651	-	-	-	X
57	MG	2A	3118	-	-	-	X
57	MG	2A	3186	-	-	-	X
57	MG	2A	3192	-	-	-	X
57	MG	2A	3310	-	-	-	X
57	MG	2A	3318	-	-	-	X
57	MG	2A	3379	-	-	-	X
57	MG	2A	3666	-	-	-	X
57	MG	2A	3746	-	-	-	X
57	MG	2A	3779	-	-	-	X
57	MG	2a	1720	-	-	-	X
57	MG	2a	1806	-	-	-	X

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 299852 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1v	13	Total	C	N	O	P	0	0	0
			286	128	59	86	13			
53	2v	13	Total	C	N	O	P	0	0	0
			286	128	59	86	13			

- Molecule 54 is a RNA chain called A-site Aminoacyl-tRNA Gly-NH-tRNAgly.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
54	1w	73	Total	C	N	O	P	S	0	0	0
			1556	695	275	512	73	1			
54	2w	72	Total	C	N	O	P	S	0	0	0
			1536	686	273	504	72	1			

- Molecule 55 is a RNA chain called P-site Aminoacyl-tRNA fMet-NH-tRNAmet.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
55	1x	77	Total	C	N	O	P	S	0	0	0
			1656	740	299	538	77	2			
55	2x	77	Total	C	N	O	P	S	0	0	0
			1656	740	299	538	77	2			

- Molecule 56 is a RNA chain called E-site Deacylated tRNAgly.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
56	1y	73	Total	C	N	O	P	S	0	0	0
			1552	693	273	512	73	1			
56	2y	73	Total	C	N	O	P	S	0	0	0
			1552	693	273	512	73	1			

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1A	1096	Total	Mg	0	0
			1096	1096		
57	1B	36	Total	Mg	0	0
			36	36		
57	1D	12	Total	Mg	0	0
			12	12		
57	1E	16	Total	Mg	0	0
			16	16		
57	1F	15	Total	Mg	0	0
			15	15		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1G	4	Total 4	Mg 4	0	0
57	1I	1	Total 1	Mg 1	0	0
57	1N	6	Total 6	Mg 6	0	0
57	1O	5	Total 5	Mg 5	0	0
57	1P	6	Total 6	Mg 6	0	0
57	1Q	7	Total 7	Mg 7	0	0
57	1R	6	Total 6	Mg 6	0	0
57	1S	3	Total 3	Mg 3	0	0
57	1T	2	Total 2	Mg 2	0	0
57	1U	9	Total 9	Mg 9	0	0
57	1V	7	Total 7	Mg 7	0	0
57	1W	7	Total 7	Mg 7	0	0
57	1X	6	Total 6	Mg 6	0	0
57	1Y	2	Total 2	Mg 2	0	0
57	1Z	2	Total 2	Mg 2	0	0
57	10	9	Total 9	Mg 9	0	0
57	11	2	Total 2	Mg 2	0	0
57	12	1	Total 1	Mg 1	0	0
57	13	5	Total 5	Mg 5	0	0
57	14	1	Total 1	Mg 1	0	0
57	15	7	Total 7	Mg 7	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	16	3	Total 3	Mg 3	0	0
57	17	5	Total 5	Mg 5	0	0
57	18	6	Total 6	Mg 6	0	0
57	19	1	Total 1	Mg 1	0	0
57	1a	224	Total 224	Mg 224	0	0
57	1b	2	Total 2	Mg 2	0	0
57	1e	2	Total 2	Mg 2	0	0
57	1f	1	Total 1	Mg 1	0	0
57	1h	1	Total 1	Mg 1	0	0
57	1l	2	Total 2	Mg 2	0	0
57	1m	2	Total 2	Mg 2	0	0
57	1n	2	Total 2	Mg 2	0	0
57	1r	1	Total 1	Mg 1	0	0
57	1t	1	Total 1	Mg 1	0	0
57	1w	9	Total 9	Mg 9	0	0
57	1x	12	Total 12	Mg 12	0	0
57	2A	861	Total 861	Mg 861	0	0
57	2B	18	Total 18	Mg 18	0	0
57	2D	7	Total 7	Mg 7	0	0
57	2E	9	Total 9	Mg 9	0	0
57	2F	6	Total 6	Mg 6	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	2G	1	Total 1	Mg 1	0	0
57	2N	1	Total 1	Mg 1	0	0
57	2O	1	Total 1	Mg 1	0	0
57	2P	2	Total 2	Mg 2	0	0
57	2Q	4	Total 4	Mg 4	0	0
57	2R	2	Total 2	Mg 2	0	0
57	2T	3	Total 3	Mg 3	0	0
57	2U	2	Total 2	Mg 2	0	0
57	2V	3	Total 3	Mg 3	0	0
57	2W	2	Total 2	Mg 2	0	0
57	2X	2	Total 2	Mg 2	0	0
57	2Y	1	Total 1	Mg 1	0	0
57	2Z	1	Total 1	Mg 1	0	0
57	20	2	Total 2	Mg 2	0	0
57	21	2	Total 2	Mg 2	0	0
57	23	3	Total 3	Mg 3	0	0
57	25	5	Total 5	Mg 5	0	0
57	26	1	Total 1	Mg 1	0	0
57	27	2	Total 2	Mg 2	0	0
57	28	3	Total 3	Mg 3	0	0
57	2a	226	Total 226	Mg 226	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	2d	2	Total 2	Mg 2	0	0
57	2e	1	Total 1	Mg 1	0	0
57	2f	1	Total 1	Mg 1	0	0
57	2g	1	Total 1	Mg 1	0	0
57	2i	1	Total 1	Mg 1	0	0
57	2j	2	Total 2	Mg 2	0	0
57	2k	1	Total 1	Mg 1	0	0
57	2l	3	Total 3	Mg 3	0	0
57	2q	2	Total 2	Mg 2	0	0
57	2r	2	Total 2	Mg 2	0	0
57	2t	1	Total 1	Mg 1	0	0
57	2v	2	Total 2	Mg 2	0	0
57	2w	4	Total 4	Mg 4	0	0
57	2x	6	Total 6	Mg 6	0	0

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

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

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

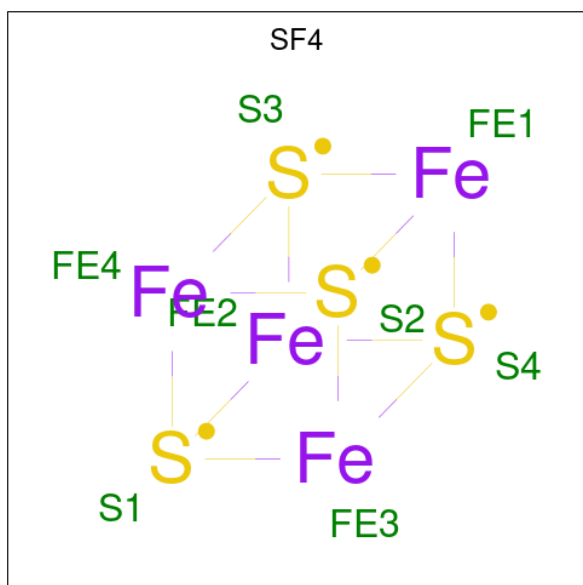
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1Y	1	Total 1	Zn 1	0	0

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

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



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

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	1984	Total	O	0	0
			1984	1984		
61	1B	63	Total	O	0	0
			63	63		
61	1D	27	Total	O	0	0
			27	27		
61	1E	27	Total	O	0	0
			27	27		
61	1F	17	Total	O	0	0
			17	17		
61	1G	4	Total	O	0	0
			4	4		
61	1H	2	Total	O	0	0
			2	2		
61	1I	1	Total	O	0	0
			1	1		
61	1N	4	Total	O	0	0
			4	4		
61	1O	5	Total	O	0	0
			5	5		
61	1P	17	Total	O	0	0
			17	17		
61	1Q	8	Total	O	0	0
			8	8		
61	1R	6	Total	O	0	0
			6	6		
61	1S	2	Total	O	0	0
			2	2		
61	1T	9	Total	O	0	0
			9	9		
61	1U	10	Total	O	0	0
			10	10		
61	1V	11	Total	O	0	0
			11	11		
61	1W	9	Total	O	0	0
			9	9		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1X	6	Total 6	O 6	0	0
61	1Y	4	Total 4	O 4	0	0
61	10	12	Total 12	O 12	0	0
61	11	8	Total 8	O 8	0	0
61	12	3	Total 3	O 3	0	0
61	13	6	Total 6	O 6	0	0
61	15	7	Total 7	O 7	0	0
61	16	4	Total 4	O 4	0	0
61	17	9	Total 9	O 9	0	0
61	18	12	Total 12	O 12	0	0
61	1a	278	Total 278	O 278	0	0
61	1b	1	Total 1	O 1	0	0
61	1d	1	Total 1	O 1	0	0
61	1e	1	Total 1	O 1	0	0
61	1f	1	Total 1	O 1	0	0
61	1i	1	Total 1	O 1	0	0
61	1l	6	Total 6	O 6	0	0
61	1m	1	Total 1	O 1	0	0
61	1o	1	Total 1	O 1	0	0
61	1q	3	Total 3	O 3	0	0
61	1u	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1v	4	Total 4	O 4	0	0
61	1w	7	Total 7	O 7	0	0
61	1x	12	Total 12	O 12	0	0
61	1y	1	Total 1	O 1	0	0
61	2A	1142	Total 1142	O 1142	0	0
61	2B	21	Total 21	O 21	0	0
61	2D	28	Total 28	O 28	0	0
61	2E	12	Total 12	O 12	0	0
61	2F	17	Total 17	O 17	0	0
61	2I	1	Total 1	O 1	0	0
61	2N	1	Total 1	O 1	0	0
61	2O	1	Total 1	O 1	0	0
61	2P	8	Total 8	O 8	0	0
61	2Q	1	Total 1	O 1	0	0
61	2R	4	Total 4	O 4	0	0
61	2T	5	Total 5	O 5	0	0
61	2U	2	Total 2	O 2	0	0
61	2W	2	Total 2	O 2	0	0
61	2X	3	Total 3	O 3	0	0
61	2Y	1	Total 1	O 1	0	0
61	2Z	1	Total 1	O 1	0	0

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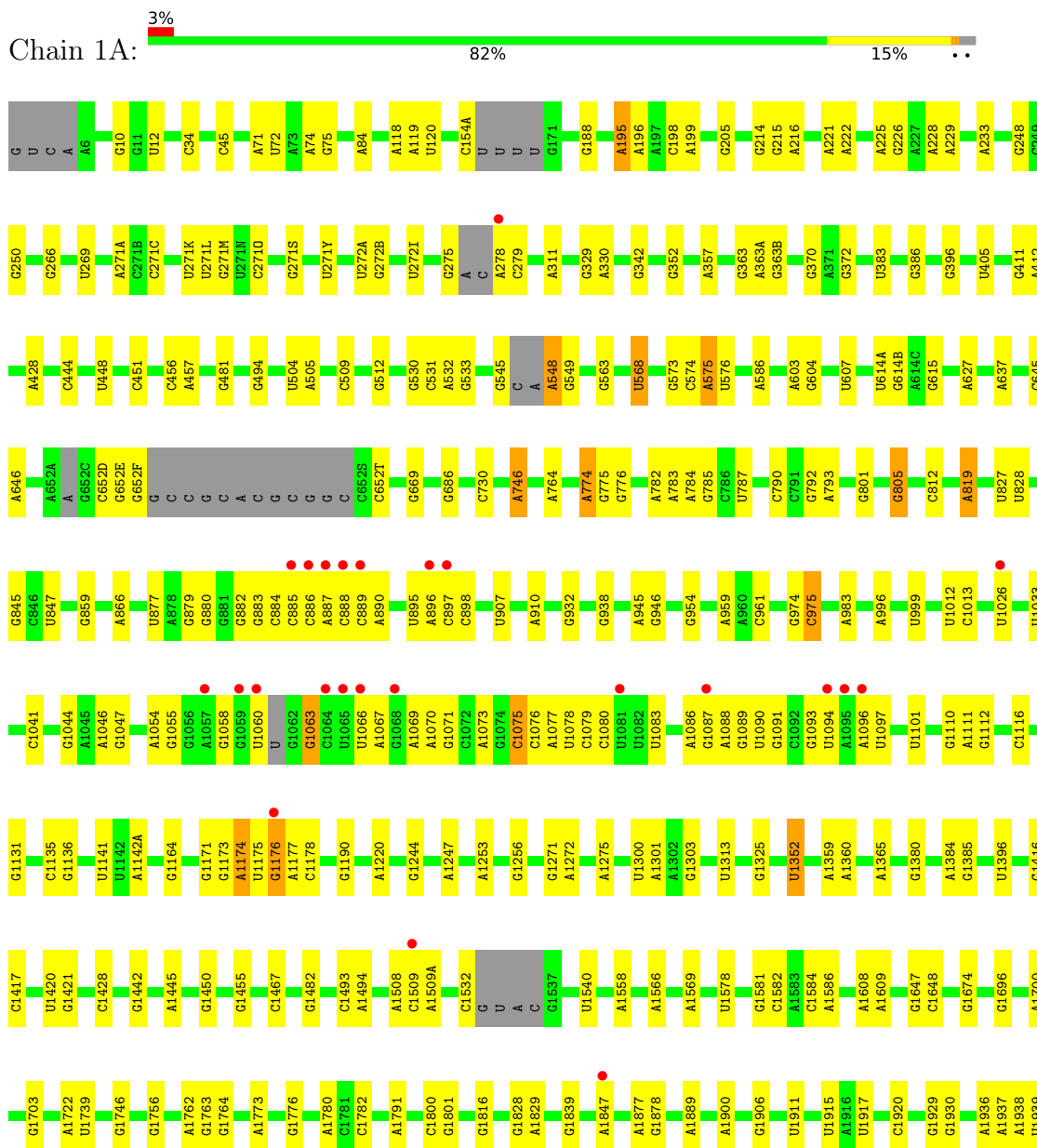
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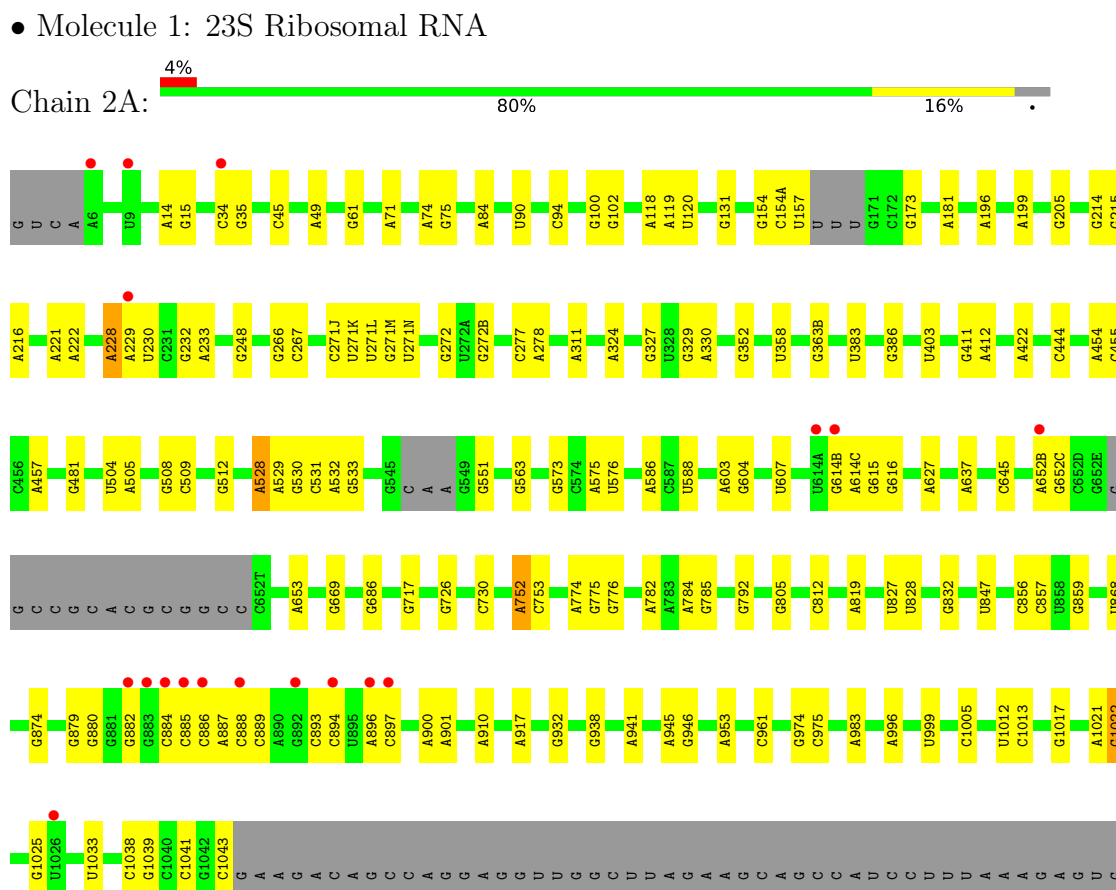
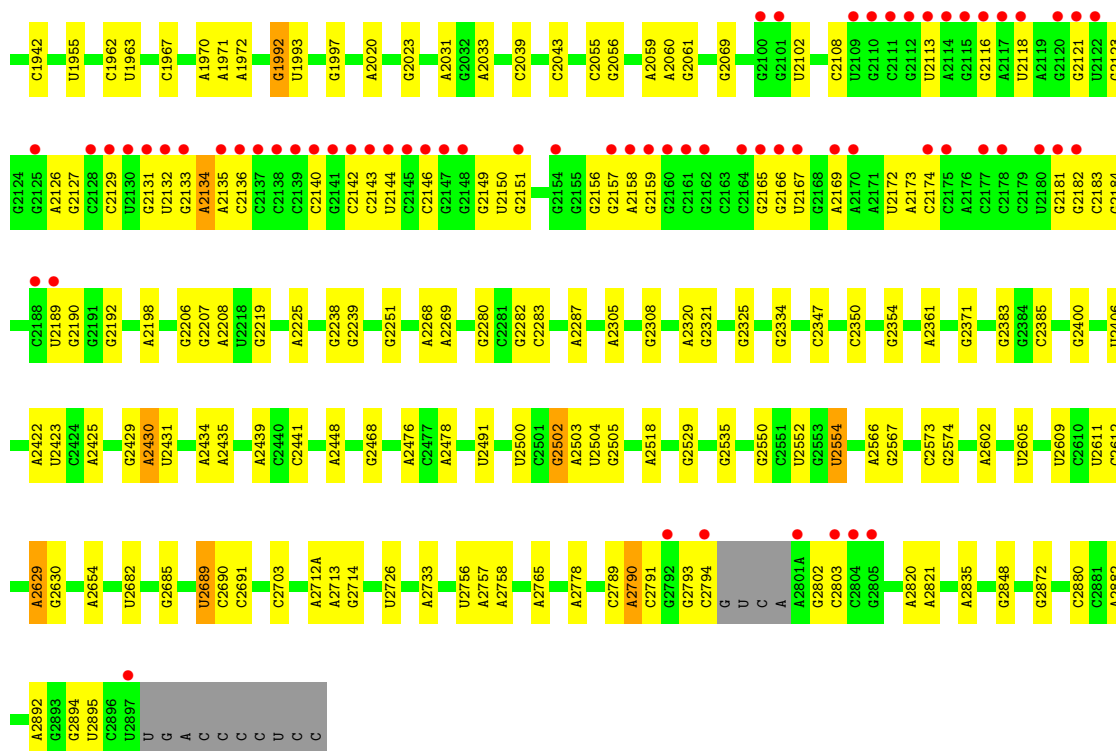
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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61	21	9	Total 9	O 9	0	0
61	23	2	Total 2	O 2	0	0
61	25	2	Total 2	O 2	0	0
61	27	4	Total 4	O 4	0	0
61	28	6	Total 6	O 6	0	0
61	29	1	Total 1	O 1	0	0
61	2a	210	Total 210	O 210	0	0
61	2d	1	Total 1	O 1	0	0
61	2g	1	Total 1	O 1	0	0
61	2i	1	Total 1	O 1	0	0
61	2j	2	Total 2	O 2	0	0
61	2l	3	Total 3	O 3	0	0
61	2p	1	Total 1	O 1	0	0
61	2q	2	Total 2	O 2	0	0
61	2r	1	Total 1	O 1	0	0
61	2t	3	Total 3	O 3	0	0
61	2v	1	Total 1	O 1	0	0
61	2w	1	Total 1	O 1	0	0
61	2x	3	Total 3	O 3	0	0

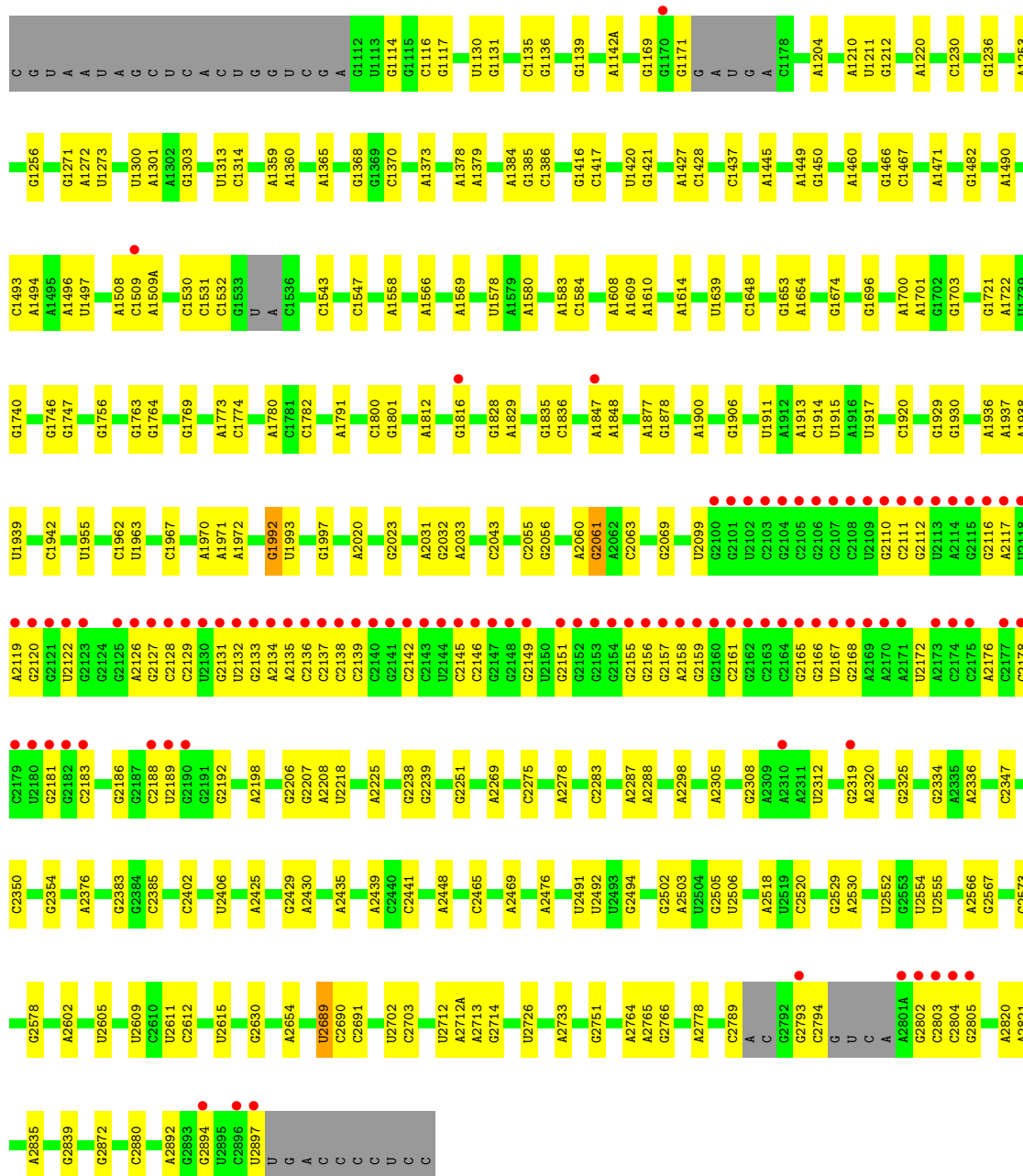
3 Residue-property plots

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

• Molecule 1: 23S Ribosomal RNA







• Molecule 2: 5S Ribosomal RNA

Chain 1B: 93% 7%

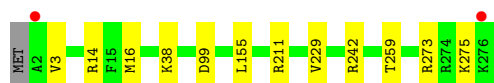


• Molecule 2: 5S Ribosomal RNA

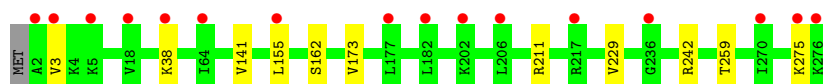
Chain 2B: 2% 79% 21%



- Molecule 3: 50S ribosomal protein L2



- Molecule 3: 50S ribosomal protein L2



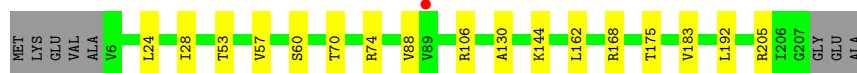
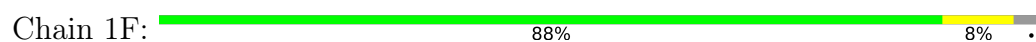
- Molecule 4: 50S ribosomal protein L3



- Molecule 4: 50S ribosomal protein L3



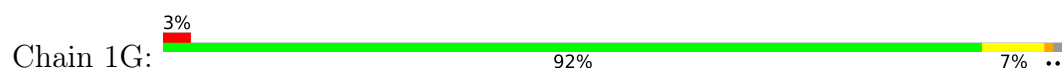
- Molecule 5: 50S ribosomal protein L4



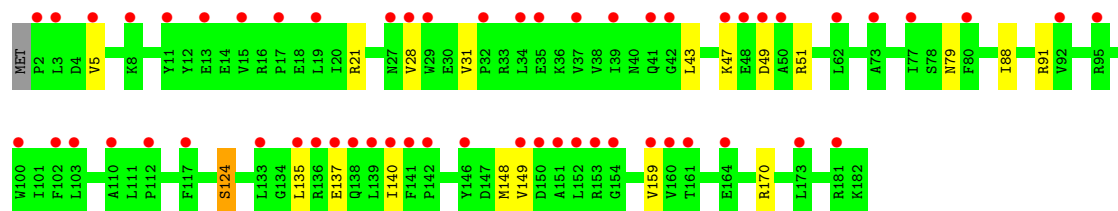
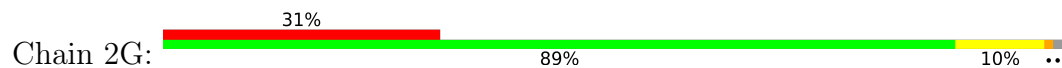
- Molecule 5: 50S ribosomal protein L4



- Molecule 6: 50S ribosomal protein L5



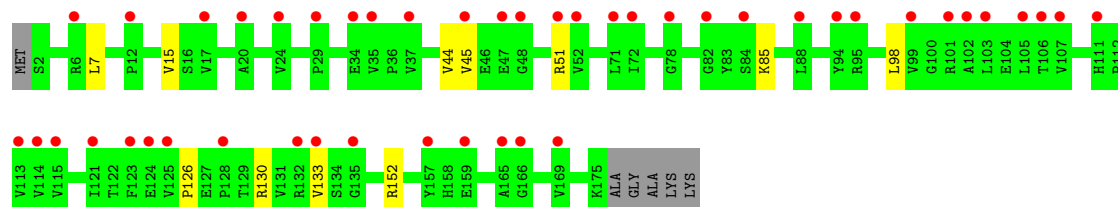
- Molecule 6: 50S ribosomal protein L5



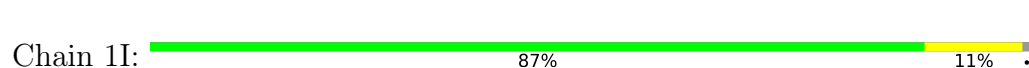
- Molecule 7: 50S ribosomal protein L6



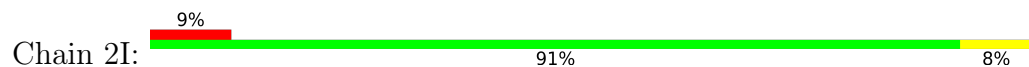
- Molecule 7: 50S ribosomal protein L6



- Molecule 8: 50S ribosomal protein L9



- Molecule 8: 50S ribosomal protein L9



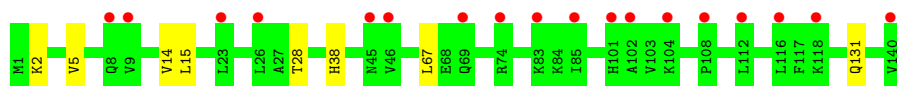
- Molecule 9: 50S ribosomal protein L13

Chain 1N:  96% .



- Molecule 9: 50S ribosomal protein L13

Chain 2N:  13% 94% 6%



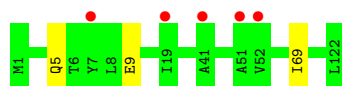
- Molecule 10: 50S ribosomal protein L14

Chain 1O:  % 98% .



- Molecule 10: 50S ribosomal protein L14

Chain 2O:  4% 98% .



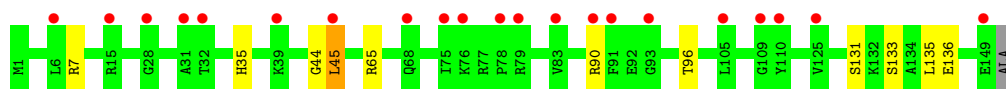
- Molecule 11: 50S ribosomal protein L15

Chain 1P:  92% 7% .



- Molecule 11: 50S ribosomal protein L15

Chain 2P:  14% 92% 7% ..

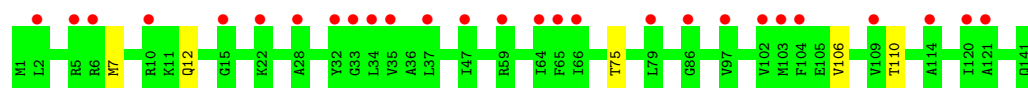


- Molecule 12: 50S ribosomal protein L16

Chain 1Q:  97% .



- Molecule 12: 50S ribosomal protein L16



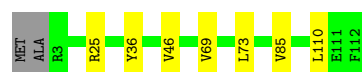
- Molecule 13: 50S ribosomal protein L17



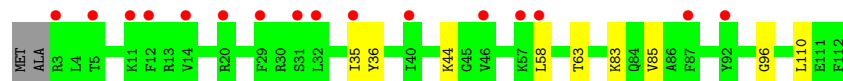
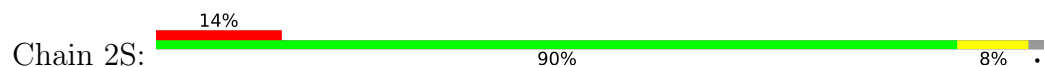
- Molecule 13: 50S ribosomal protein L17



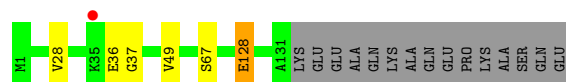
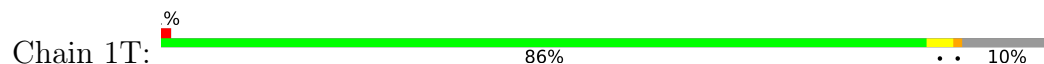
- Molecule 14: 50S ribosomal protein L18



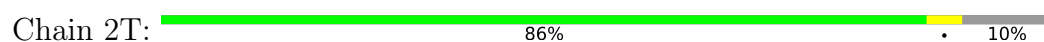
- Molecule 14: 50S ribosomal protein L18



- Molecule 15: 50S ribosomal protein L19



- Molecule 15: 50S ribosomal protein L19



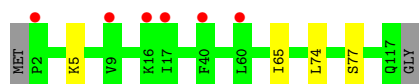
- Molecule 16: 50S ribosomal protein L20

Chain 1U:  96% ..



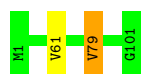
- Molecule 16: 50S ribosomal protein L20

Chain 2U:  5% 95% ..



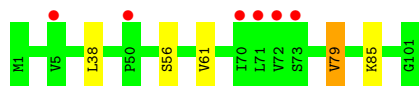
- Molecule 17: 50S ribosomal protein L21

Chain 1V:  98% ..



- Molecule 17: 50S ribosomal protein L21

Chain 2V:  6% 95% ..



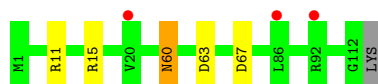
- Molecule 18: 50S ribosomal protein L22

Chain 1W:  96% ..



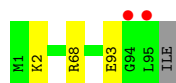
- Molecule 18: 50S ribosomal protein L22

Chain 2W:  3% 95% ..



- Molecule 19: 50S ribosomal protein L23

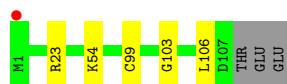
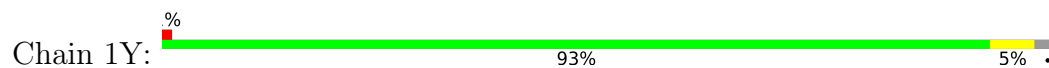
Chain 1X:  2% 96% ..



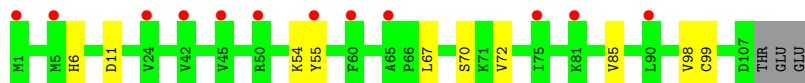
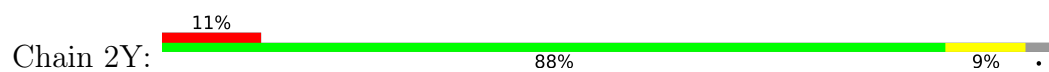
- Molecule 19: 50S ribosomal protein L23



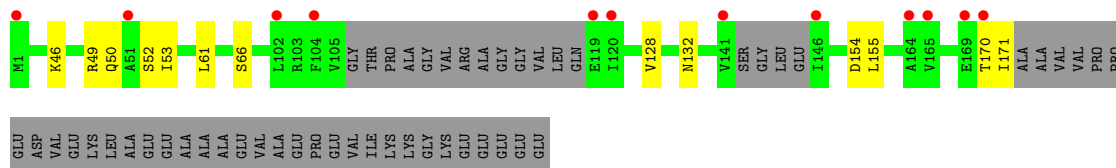
- Molecule 20: 50S ribosomal protein L24



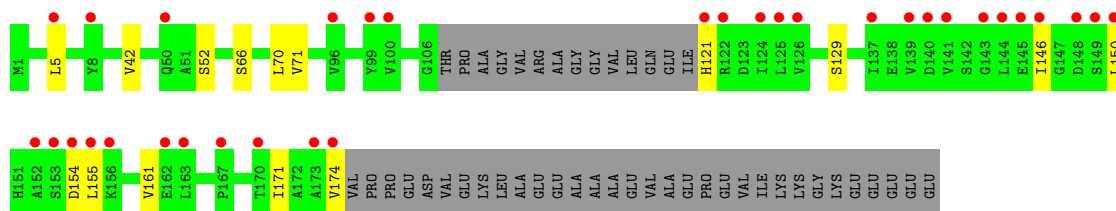
- Molecule 20: 50S ribosomal protein L24



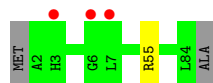
- Molecule 21: 50S ribosomal protein L25



- Molecule 21: 50S ribosomal protein L25



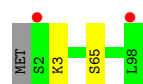
- Molecule 22: 50S ribosomal protein L27



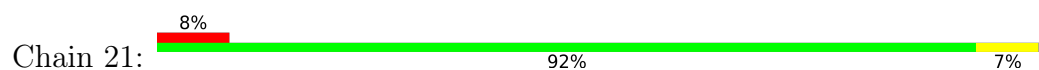
- Molecule 22: 50S ribosomal protein L27



- Molecule 23: 50S ribosomal protein L28



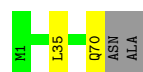
- Molecule 23: 50S ribosomal protein L28



- Molecule 24: 50S ribosomal protein L29



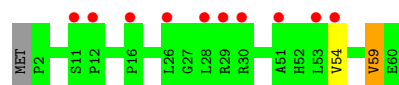
- Molecule 24: 50S ribosomal protein L29



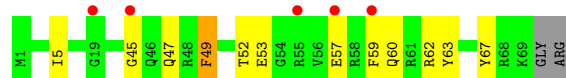
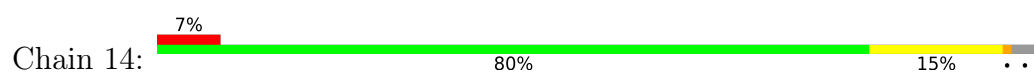
- Molecule 25: 50S ribosomal protein L30



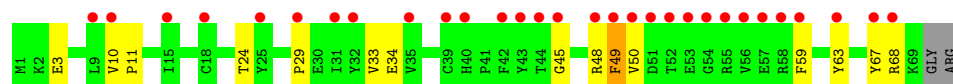
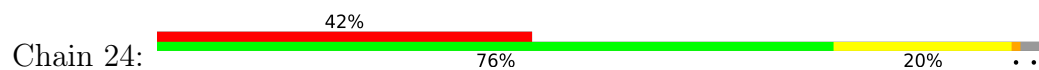
- Molecule 25: 50S ribosomal protein L30



- Molecule 26: 50S ribosomal protein L31



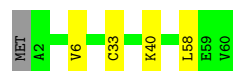
- Molecule 26: 50S ribosomal protein L31



- Molecule 27: 50S ribosomal protein L32



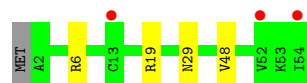
- Molecule 27: 50S ribosomal protein L32



- Molecule 28: 50S ribosomal protein L33



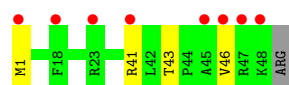
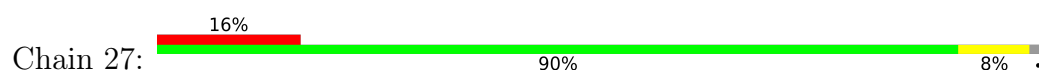
- Molecule 28: 50S ribosomal protein L33



- Molecule 29: 50S ribosomal protein L34



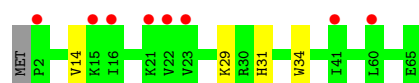
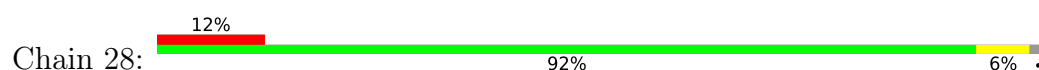
- Molecule 29: 50S ribosomal protein L34



- Molecule 30: 50S ribosomal protein L35



- Molecule 30: 50S ribosomal protein L35

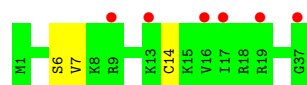


- Molecule 31: 50S ribosomal protein L36

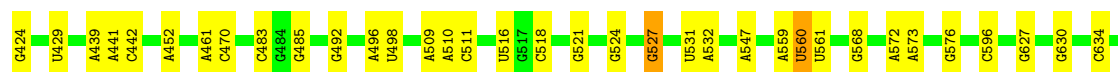
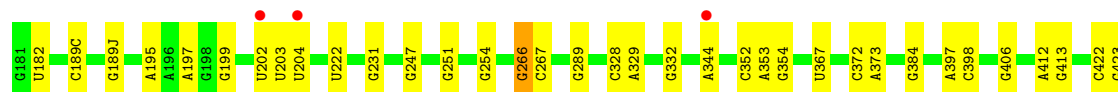
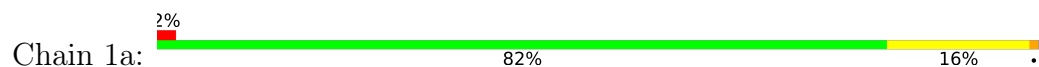


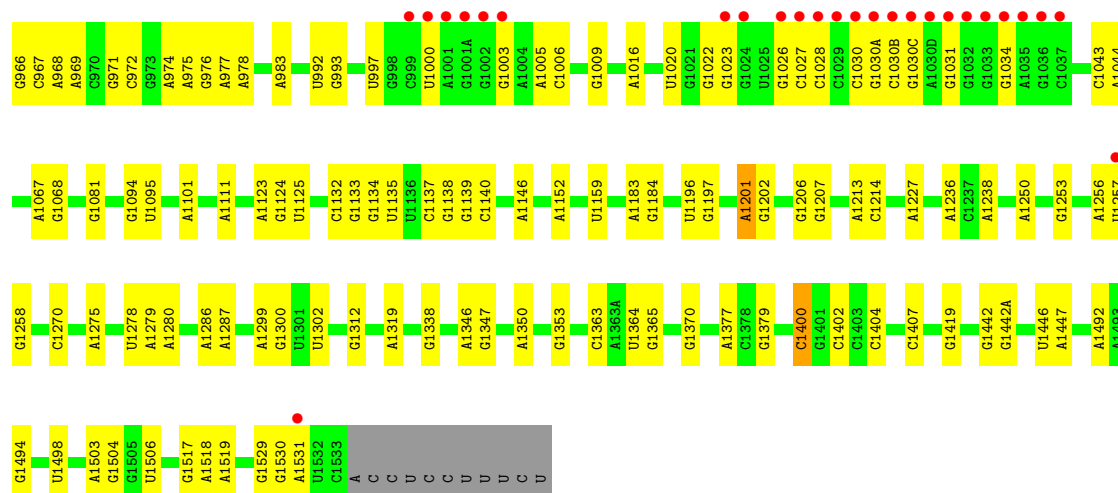
There are no outlier residues recorded for this chain.

- Molecule 31: 50S ribosomal protein L36

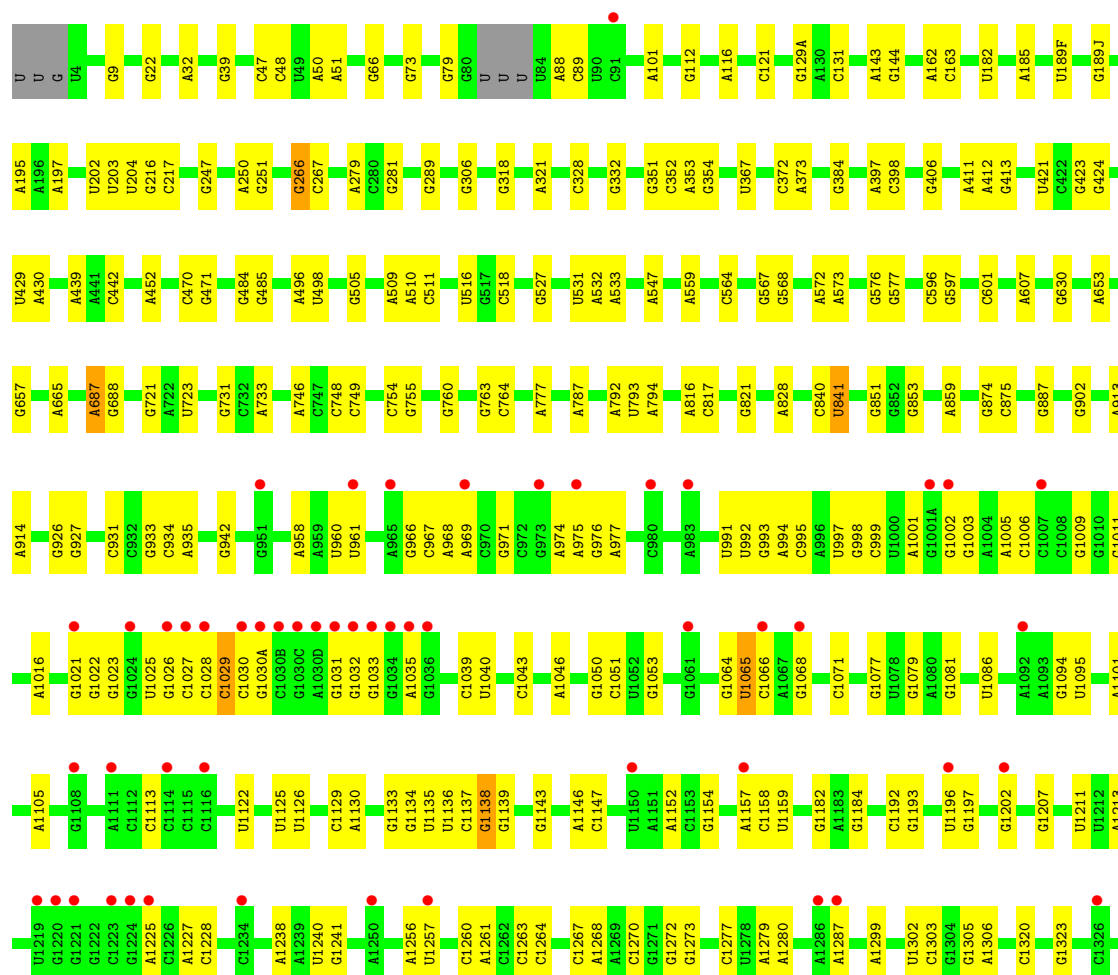
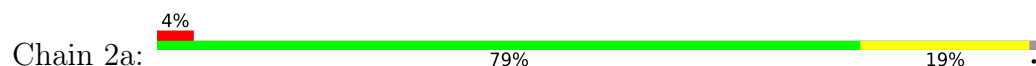


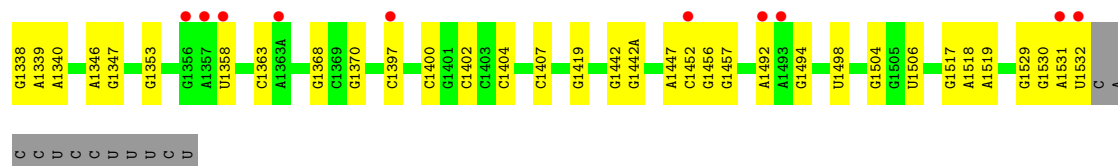
- Molecule 32: 16S Ribosomal RNA



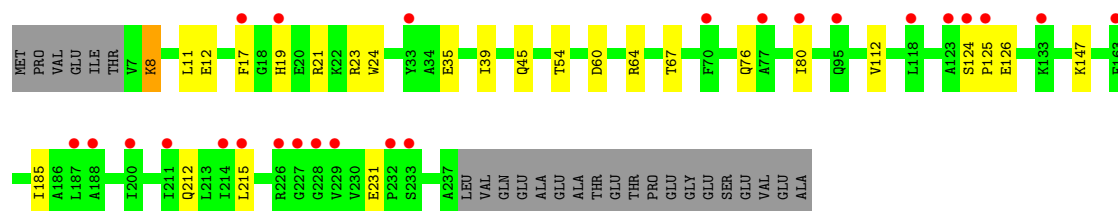
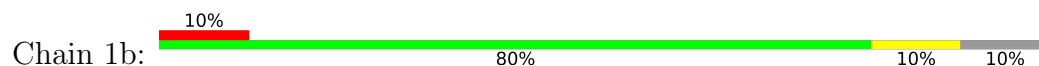


- Molecule 32: 16S Ribosomal RNA

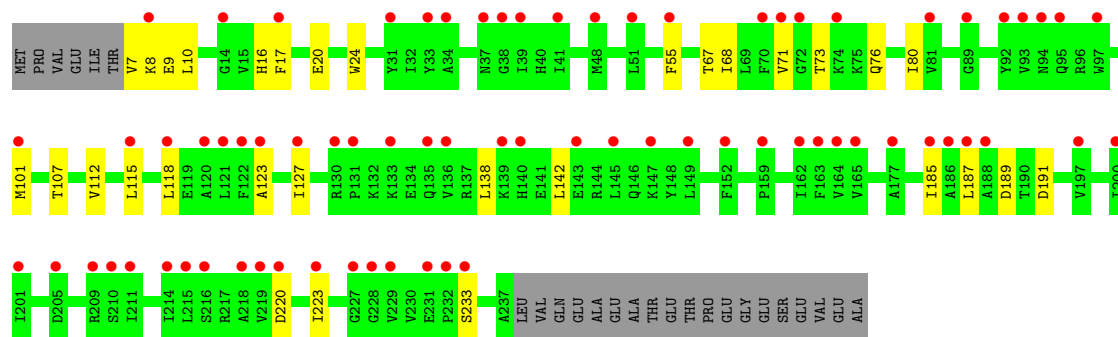
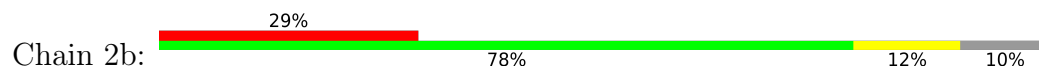




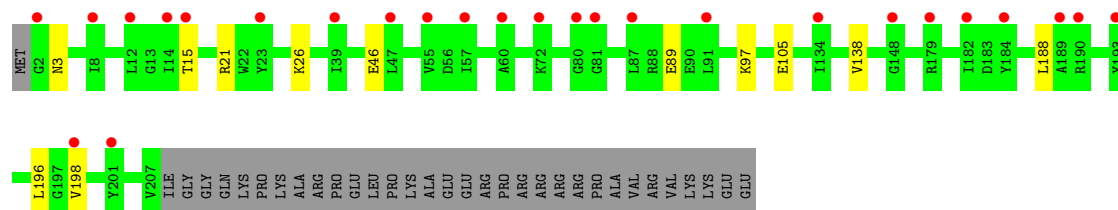
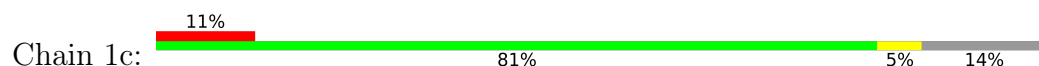
• Molecule 33: 30S ribosomal protein S2



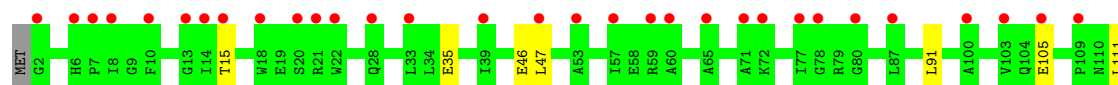
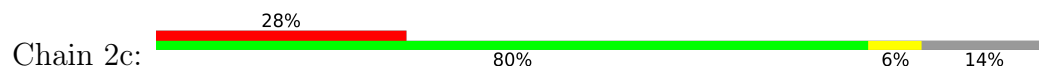
• Molecule 33: 30S ribosomal protein S2

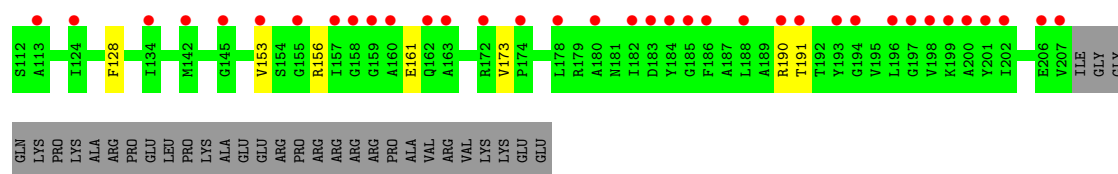


• Molecule 34: 30S ribosomal protein S3

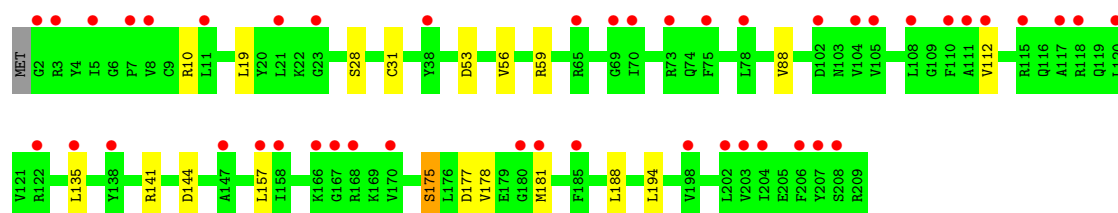


• Molecule 34: 30S ribosomal protein S3

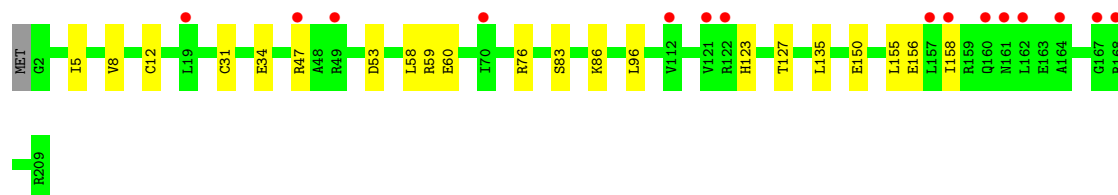
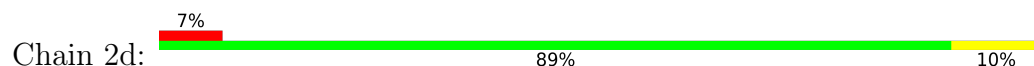




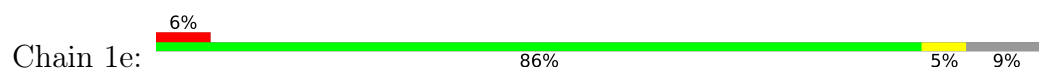
• Molecule 35: 30S ribosomal protein S4



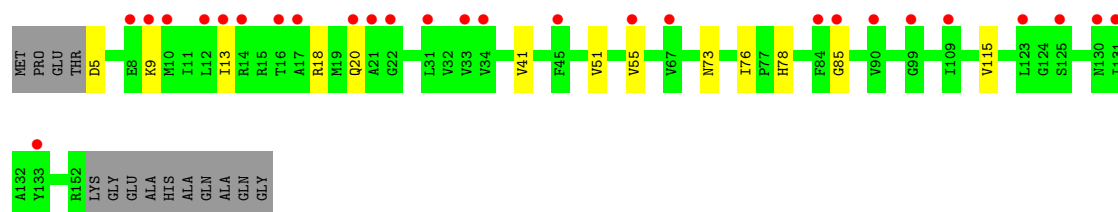
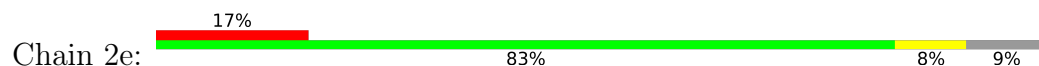
• Molecule 35: 30S ribosomal protein S4



• Molecule 36: 30S ribosomal protein S5

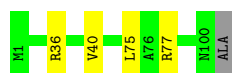


• Molecule 36: 30S ribosomal protein S5

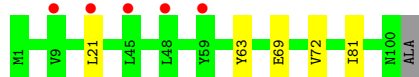


• Molecule 37: 30S ribosomal protein S6

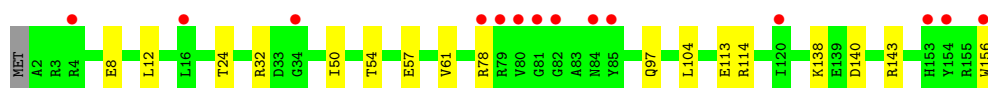
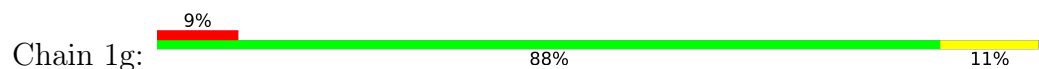




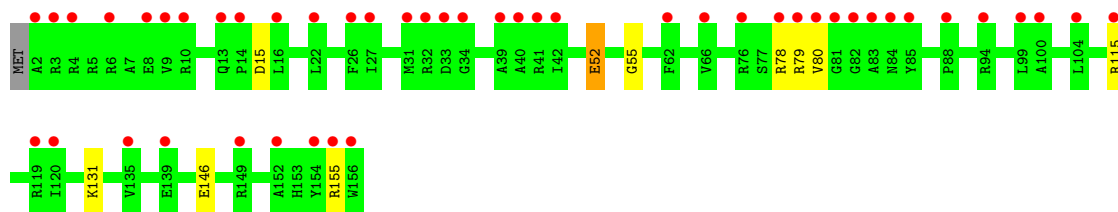
- Molecule 37: 30S ribosomal protein S6



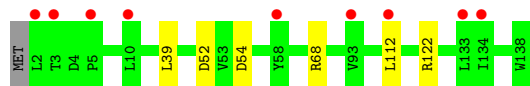
- Molecule 38: 30S ribosomal protein S7



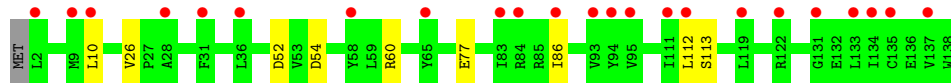
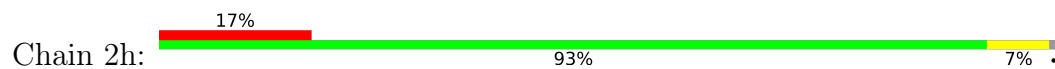
- Molecule 38: 30S ribosomal protein S7



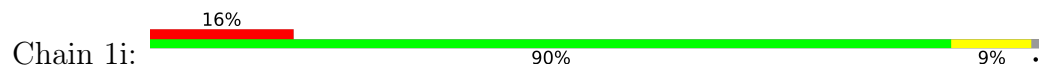
- Molecule 39: 30S ribosomal protein S8

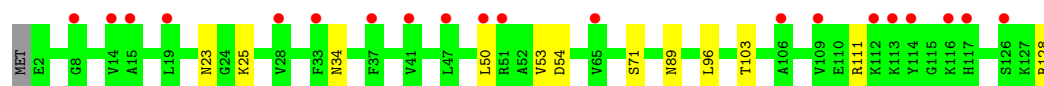


- Molecule 39: 30S ribosomal protein S8

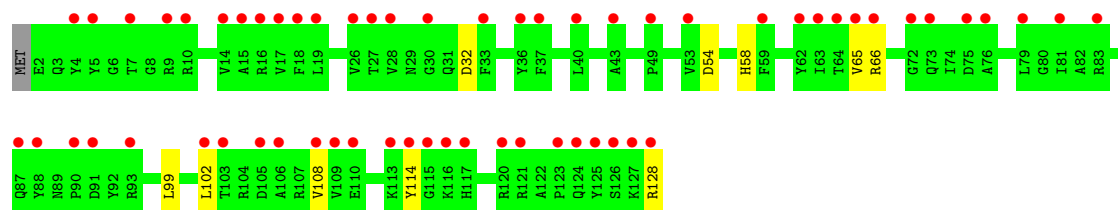
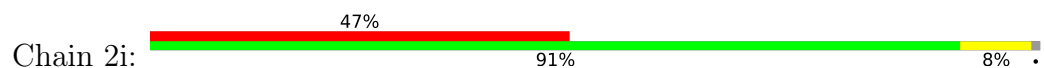


- Molecule 40: 30S ribosomal protein S9

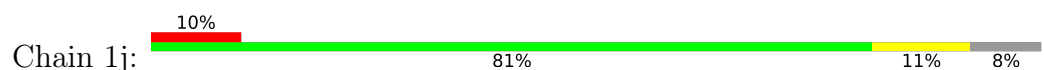




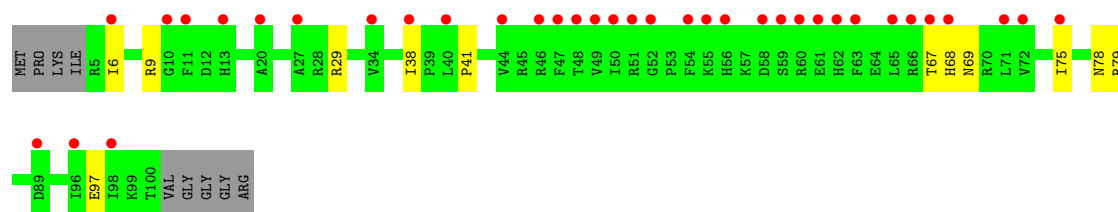
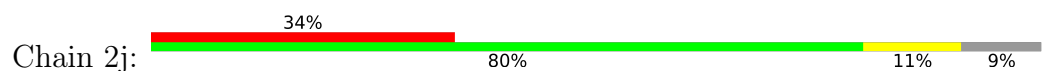
- Molecule 40: 30S ribosomal protein S9



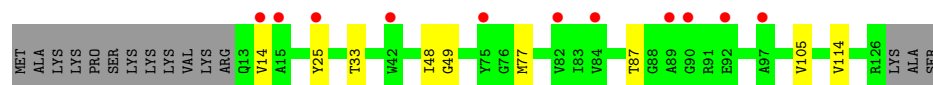
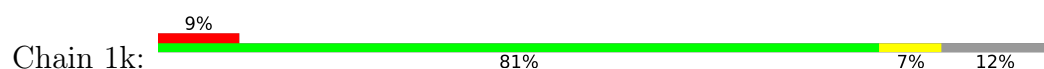
- Molecule 41: 30S ribosomal protein S10



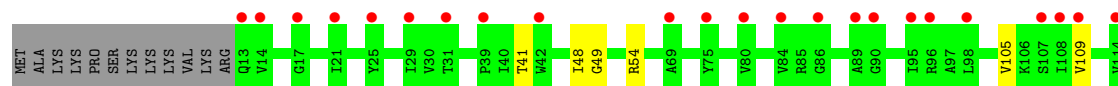
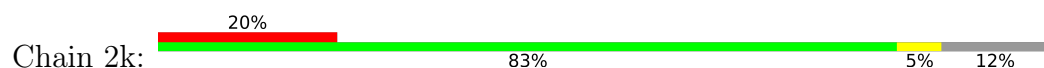
- Molecule 41: 30S ribosomal protein S10

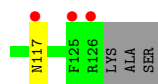


- Molecule 42: 30S ribosomal protein S11

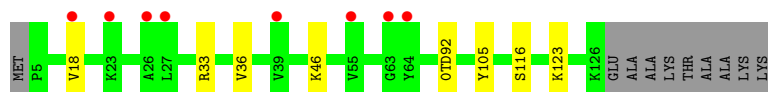
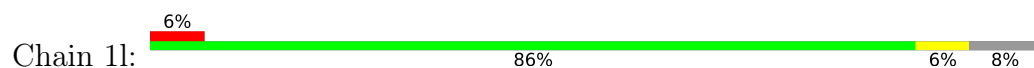


- Molecule 42: 30S ribosomal protein S11

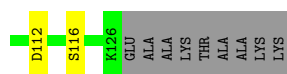
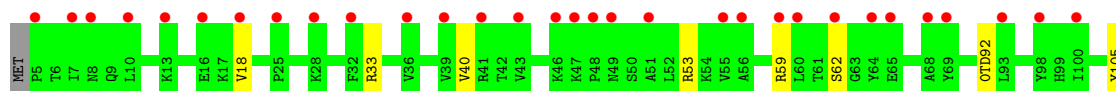
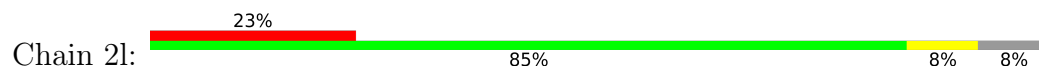




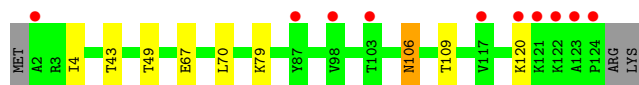
- Molecule 43: 30S ribosomal protein S12



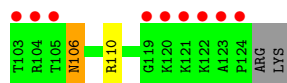
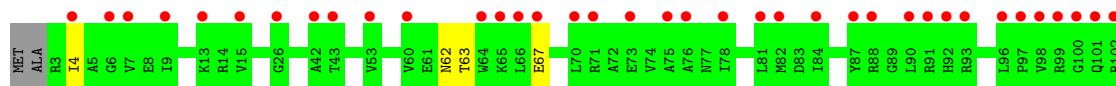
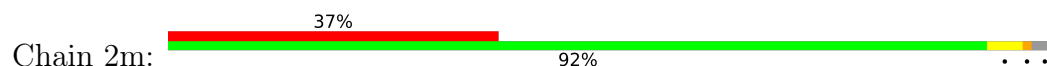
- Molecule 43: 30S ribosomal protein S12



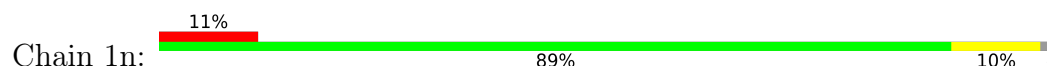
- Molecule 44: 30S ribosomal protein S13



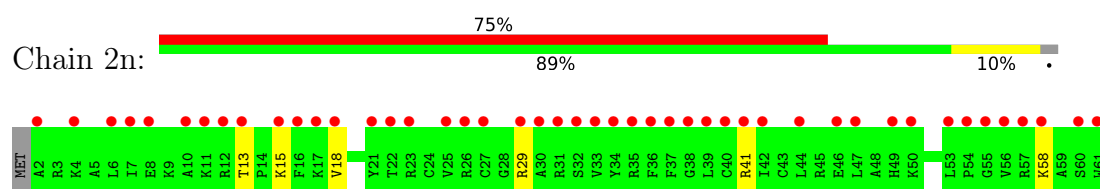
- Molecule 44: 30S ribosomal protein S13



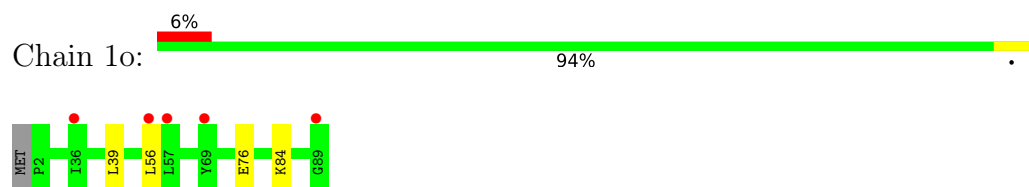
- Molecule 45: 30S ribosomal protein S14 type Z



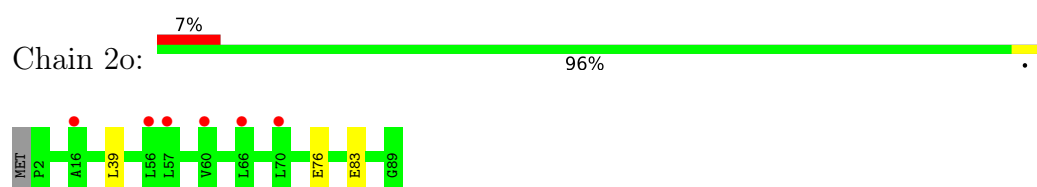
- Molecule 45: 30S ribosomal protein S14 type Z



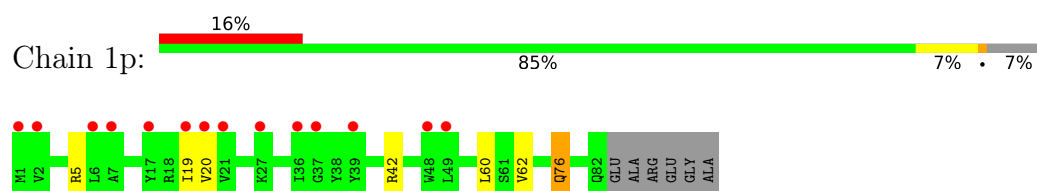
- Molecule 46: 30S ribosomal protein S15



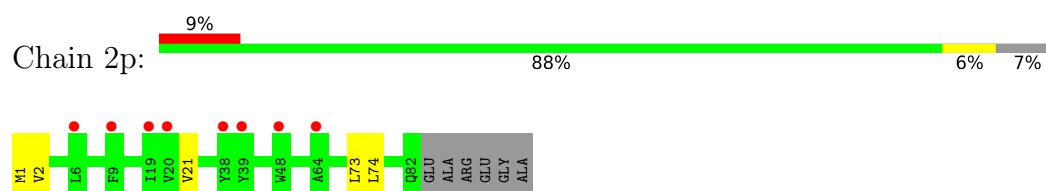
- Molecule 46: 30S ribosomal protein S15



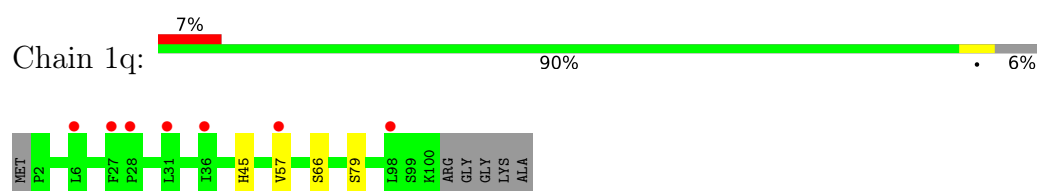
- Molecule 47: 30S ribosomal protein S16



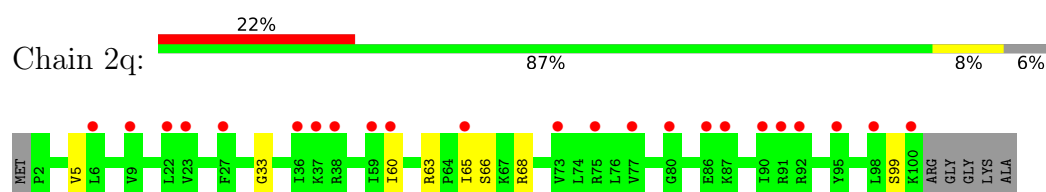
- Molecule 47: 30S ribosomal protein S16



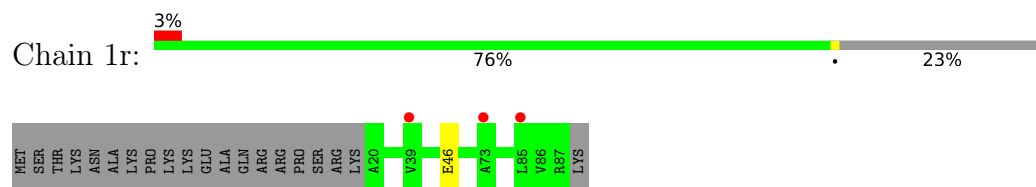
- Molecule 48: 30S ribosomal protein S17



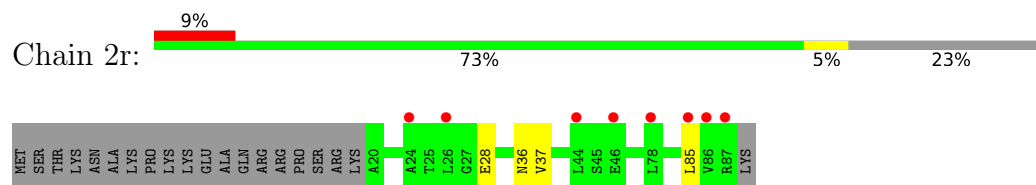
- Molecule 48: 30S ribosomal protein S17



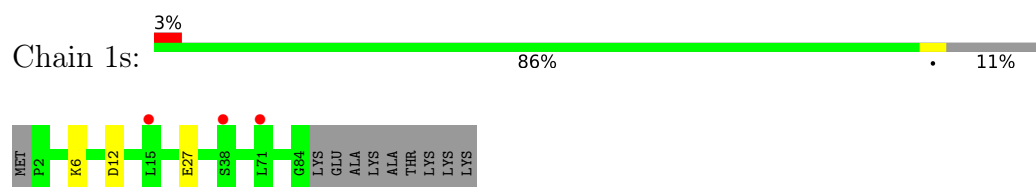
- Molecule 49: 30S ribosomal protein S18



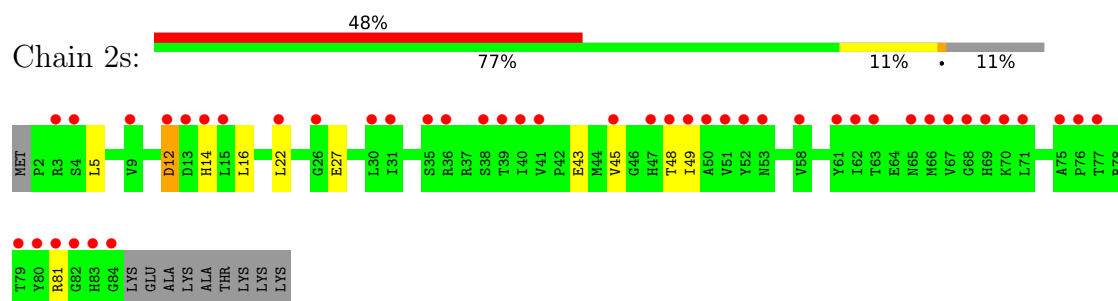
- Molecule 49: 30S ribosomal protein S18



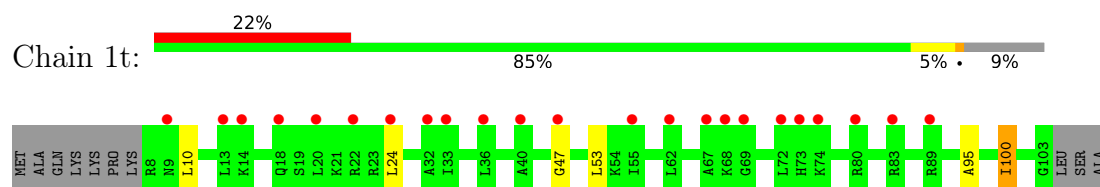
- Molecule 50: 30S ribosomal protein S19



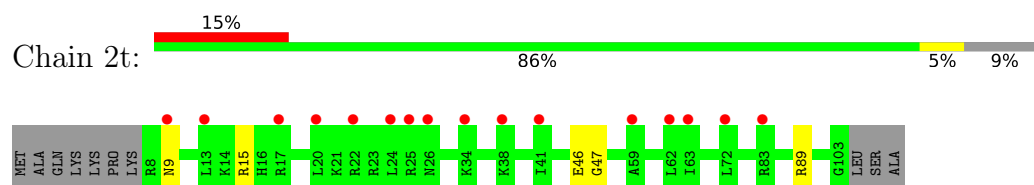
- Molecule 50: 30S ribosomal protein S19



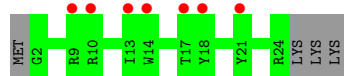
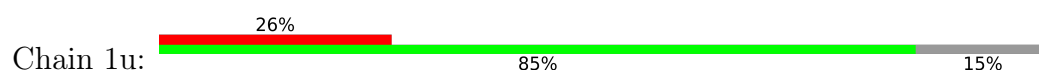
- Molecule 51: 30S ribosomal protein S20



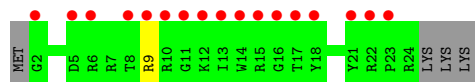
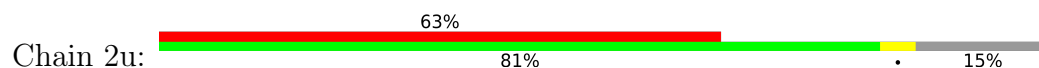
- Molecule 51: 30S ribosomal protein S20



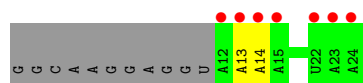
- Molecule 52: 30S ribosomal protein Thx



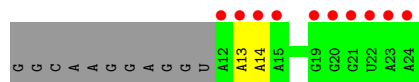
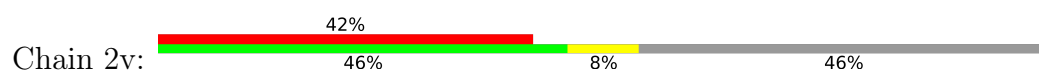
- Molecule 52: 30S ribosomal protein Thx



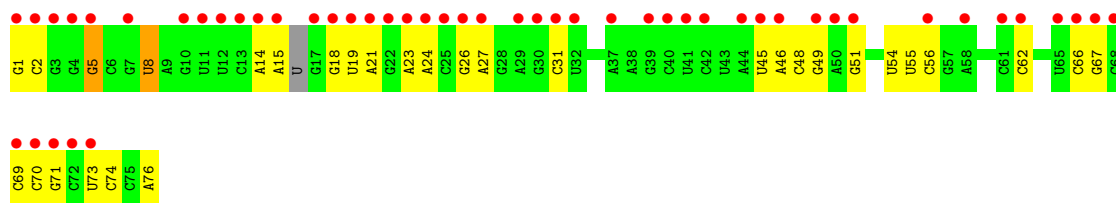
- Molecule 53: MG-mRNA



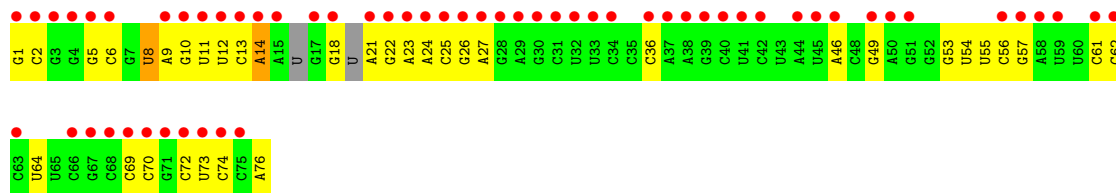
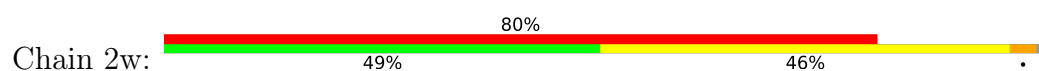
- Molecule 53: MG-mRNA



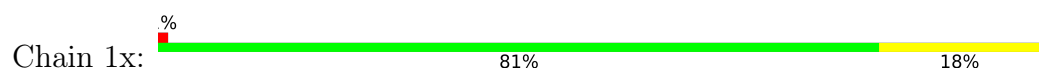
- Molecule 54: A-site Aminoacyl-tRNA Gly-NH-tRNAgly



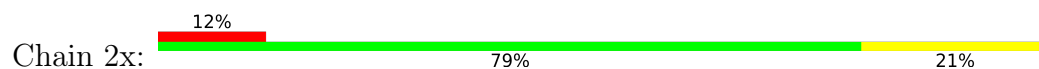
- Molecule 54: A-site Aminoacyl-tRNA Gly-NH-tRNAgly



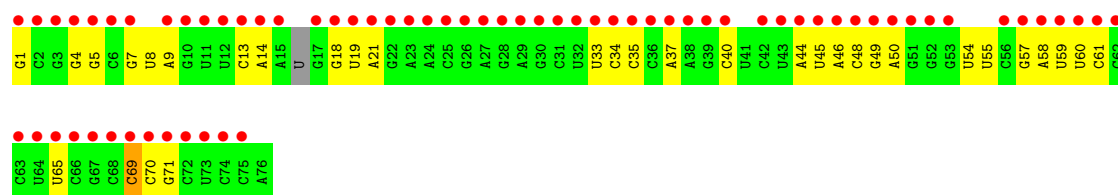
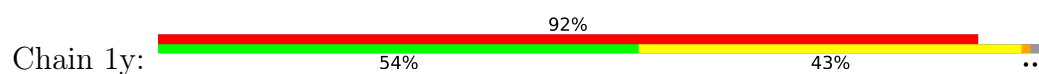
- Molecule 55: P-site Aminoacyl-tRNA fMet-NH-tRNAmet



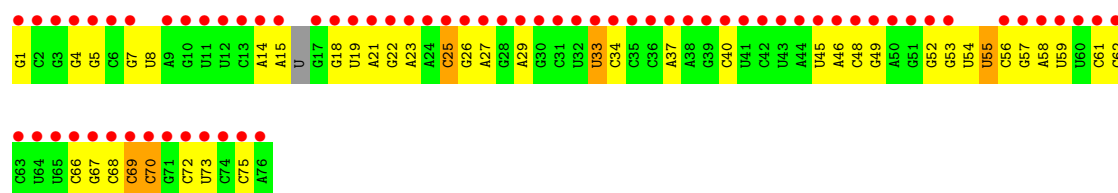
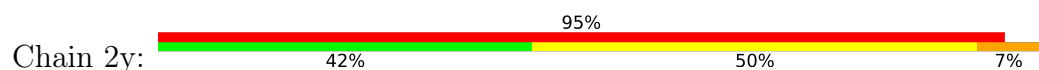
- Molecule 55: P-site Aminoacyl-tRNA fMet-NH-tRNA^{Met}



- Molecule 56: E-site Deacylated tRNA^{Gly}



- Molecule 56: E-site Deacylated tRNA^{Gly}



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.61Å 451.44Å 624.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	146.30 – 2.55 225.72 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.4 (146.30-2.55) 99.4 (225.72-2.55)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 2.55Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.220 , 0.263 0.220 , 0.263	Depositor DCC
R_{free} test set	95245 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	50.7	Xtriage
Anisotropy	0.191	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 54.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	299852	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, L3X, MG, 2MA, 2MG, 4OC, G7M, OMU, UR3, M2G, 4SU, MA6, 5MU, ZN, 5MC, 31H, OMC, OMG, PSU, 0TD, K

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	0.49	0/69011	0.97	69/107720 (0.1%)
1	2A	0.38	0/67295	0.87	26/105042 (0.0%)
2	1B	0.43	1/2882 (0.0%)	0.86	0/4494
2	2B	0.39	1/2879 (0.0%)	0.83	1/4487 (0.0%)
3	1D	0.35	0/2186	0.56	0/2944
3	2D	0.30	0/2186	0.51	0/2944
4	1E	0.33	0/1592	0.55	0/2149
4	2E	0.29	0/1592	0.51	0/2149
5	1F	0.33	0/1618	0.54	0/2191
5	2F	0.29	0/1614	0.49	0/2186
6	1G	0.29	0/1448	0.49	0/1957
6	2G	0.29	0/1453	0.47	0/1963
7	1H	0.31	0/1356	0.50	0/1834
7	2H	0.27	0/1356	0.47	0/1834
8	1I	0.28	0/1112	0.47	0/1514
8	2I	0.27	0/1079	0.48	0/1475
9	1N	0.33	0/1144	0.50	0/1543
9	2N	0.29	0/1144	0.44	0/1543
10	1O	0.33	0/943	0.52	0/1269
10	2O	0.29	0/943	0.51	0/1269
11	1P	0.33	0/1152	0.58	0/1533
11	2P	0.31	0/1152	0.53	0/1533
12	1Q	0.34	0/1143	0.52	0/1527
12	2Q	0.30	0/1143	0.48	0/1527
13	1R	0.32	0/982	0.53	0/1312
13	2R	0.27	0/982	0.51	0/1312
14	1S	0.31	0/883	0.51	0/1176
14	2S	0.30	0/880	0.48	0/1172
15	1T	0.32	0/1105	0.51	0/1477
15	2T	0.28	0/1097	0.47	0/1468
16	1U	0.34	0/977	0.50	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.29	0/977	0.45	0/1301
17	1V	0.37	0/782	0.55	0/1049
17	2V	0.30	0/782	0.48	0/1049
18	1W	0.36	0/897	0.51	0/1205
18	2W	0.30	0/897	0.49	0/1205
19	1X	0.36	0/764	0.56	0/1025
19	2X	0.29	0/764	0.51	0/1025
20	1Y	0.33	0/819	0.52	0/1095
20	2Y	0.30	0/819	0.51	0/1095
21	1Z	0.29	0/1267	0.51	0/1717
21	2Z	0.31	0/1299	0.48	0/1763
22	10	0.34	0/662	0.52	0/881
22	20	0.30	0/662	0.50	0/881
23	11	0.32	0/762	0.54	0/1014
23	21	0.31	0/762	0.51	0/1014
24	12	0.30	0/590	0.48	0/781
24	22	0.27	0/590	0.40	0/781
25	13	0.31	0/474	0.53	0/635
25	23	0.26	0/469	0.45	0/630
26	14	0.31	0/565	0.57	0/761
26	24	0.33	0/545	0.49	0/737
27	15	0.33	0/469	0.55	0/635
27	25	0.30	0/469	0.50	0/635
28	16	0.33	0/460	0.51	0/613
28	26	0.28	0/456	0.49	0/608
29	17	0.34	0/426	0.54	0/561
29	27	0.28	0/426	0.51	0/561
30	18	0.30	0/525	0.55	0/691
30	28	0.27	0/525	0.48	0/691
31	19	0.35	0/310	0.53	0/407
31	29	0.28	0/310	0.52	0/407
32	1a	0.36	0/35795	0.87	21/55864 (0.0%)
32	2a	0.35	2/35886 (0.0%)	0.87	35/56005 (0.1%)
33	1b	0.30	0/1881	0.49	0/2542
33	2b	0.30	0/1860	0.48	0/2518
34	1c	0.29	0/1572	0.47	0/2126
34	2c	0.30	0/1566	0.48	0/2119
35	1d	0.28	0/1685	0.46	0/2262
35	2d	0.27	0/1704	0.45	0/2284
36	1e	0.29	0/1145	0.49	0/1543
36	2e	0.29	0/1149	0.49	0/1548
37	1f	0.29	0/823	0.47	0/1115
37	2f	0.28	0/829	0.48	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	0.27	0/1108	0.45	0/1494
40	1i	0.28	0/1002	0.50	0/1346
40	2i	0.30	0/997	0.51	0/1343
41	1j	0.26	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	0.28	0/937	0.50	0/1260
43	2l	0.27	0/937	0.48	0/1260
44	1m	0.29	0/969	0.47	0/1302
44	2m	0.27	0/961	0.48	0/1291
45	1n	0.28	0/501	0.47	0/664
45	2n	0.29	0/501	0.47	0/664
46	1o	0.28	0/739	0.43	0/985
46	2o	0.26	0/739	0.43	0/985
47	1p	0.27	0/697	0.53	0/939
47	2p	0.26	0/693	0.49	0/935
48	1q	0.28	0/836	0.49	0/1117
48	2q	0.28	0/836	0.46	0/1117
49	1r	0.26	0/560	0.51	0/746
49	2r	0.27	0/560	0.42	0/746
50	1s	0.27	0/667	0.51	0/900
50	2s	0.30	0/661	0.57	0/893
51	1t	0.27	0/730	0.44	0/965
51	2t	0.26	0/729	0.41	0/965
52	1u	0.25	0/203	0.49	0/266
52	2u	0.27	0/203	0.46	0/266
53	1v	0.45	0/322	0.81	0/501
53	2v	0.44	0/322	0.83	0/501
54	1w	0.54	1/1639 (0.1%)	1.11	6/2548 (0.2%)
54	2w	0.57	1/1616 (0.1%)	1.12	8/2510 (0.3%)
55	1x	0.57	1/1723 (0.1%)	1.11	15/2684 (0.6%)
55	2x	0.51	1/1723 (0.1%)	1.03	9/2684 (0.3%)
56	1y	0.58	1/1664 (0.1%)	1.11	1/2587 (0.0%)
56	2y	0.61	1/1664 (0.1%)	1.25	13/2587 (0.5%)
All	All	0.39	10/316940 (0.0%)	0.82	204/474518 (0.0%)

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

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
11	1P	0	1
11	2P	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	-10.38	1.48	1.61
2	2B	1	U	OP3-P	-10.25	1.48	1.61
2	1B	1	U	OP3-P	-10.22	1.48	1.61
54	1w	1	G	OP3-P	-10.17	1.49	1.61
56	2y	1	G	OP3-P	-10.15	1.49	1.61
56	1y	1	G	OP3-P	-10.15	1.49	1.61
54	2w	1	G	OP3-P	-10.09	1.49	1.61
55	2x	1	C	OP3-P	-10.04	1.49	1.61
32	2a	1272	G	C6-N1	-7.14	1.34	1.39
32	2a	1272	G	N1-C2	-7.11	1.32	1.37

All (204) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1263	C	N1-C2-O2	18.87	130.22	118.90
32	2a	1272	G	N3-C2-N2	18.66	132.96	119.90
32	2a	1272	G	N1-C2-N2	-16.48	101.37	116.20
32	2a	1272	G	C5-C6-O6	15.60	137.96	128.60
32	2a	1263	C	C2-N3-C4	11.89	125.84	119.90
1	2A	2136	C	N1-C2-O2	10.92	125.45	118.90
55	1x	46	G	C6-N1-C2	-10.27	118.94	125.10
32	2a	1263	C	N3-C2-O2	-10.21	114.75	121.90
54	2w	14	A	C5-C6-N6	-10.13	115.59	123.70
32	2a	1272	G	C6-N1-C2	9.97	131.08	125.10
32	2a	1272	G	C5-C6-N1	-9.77	106.61	111.50
55	1x	14	A	C4-C5-C6	9.69	121.84	117.00
1	1A	1075	C	N1-C2-O2	9.53	124.62	118.90
55	1x	14	A	C5-N7-C8	9.34	108.57	103.90
32	2a	1263	C	C5-C6-N1	9.14	125.57	121.00
32	1a	1030(B)	C	C2-N1-C1'	9.10	128.81	118.80
32	1a	1030(B)	C	N1-C2-O2	8.82	124.19	118.90
54	2w	14	A	N1-C6-N6	8.71	123.83	118.60
1	2A	1639	U	O5'-P-OP2	-8.69	97.88	105.70
1	1A	975	C	N1-C2-O2	-8.41	113.85	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	2x	46	G	C6-N1-C2	-8.38	120.08	125.10
1	1A	512	G	O4'-C1'-N9	8.22	114.78	108.20
32	2a	1272	G	C4-N9-C1'	8.21	137.17	126.50
1	1A	801	G	O5'-P-OP2	-8.12	98.39	105.70
1	1A	793	A	O5'-P-OP2	-8.04	98.46	105.70
2	2B	80	U	O4'-C1'-N1	8.00	114.60	108.20
1	1A	1075	C	C2-N3-C4	7.97	123.89	119.90
1	1A	1776	G	O5'-P-OP2	-7.87	98.61	105.70
32	2a	1272	G	C8-N9-C1'	-7.80	116.86	127.00
55	1x	22	G	C5-N7-C8	-7.50	100.55	104.30
1	1A	1063	G	C5-C6-O6	7.50	133.10	128.60
32	2a	1272	G	N1-C6-O6	-7.48	115.41	119.90
1	1A	2689	U	P-O3'-C3'	7.38	128.56	119.70
32	1a	1030(B)	C	C6-N1-C2	-7.37	117.35	120.30
1	2A	2155	G	N3-C2-N2	7.35	125.05	119.90
1	1A	576	U	O5'-P-OP1	-7.34	99.10	105.70
32	2a	1272	G	C2-N3-C4	-7.27	108.27	111.90
32	1a	1030(B)	C	N3-C2-O2	-7.18	116.87	121.90
32	2a	79	G	C5-C6-O6	7.13	132.88	128.60
32	2a	1263	C	C2-N1-C1'	7.12	126.64	118.80
55	2x	14	A	C5-N7-C8	7.12	107.46	103.90
1	1A	226	G	O4'-C1'-N9	7.09	113.87	108.20
55	2x	14	A	C4-C5-C6	7.05	120.53	117.00
1	1A	787	U	O5'-P-OP1	-6.99	99.41	105.70
56	2y	70	C	N1-C2-O2	6.93	123.06	118.90
32	2a	754	C	C2-N1-C1'	6.93	126.42	118.80
55	1x	46	G	N3-C2-N2	-6.89	115.08	119.90
56	2y	69	C	N1-C2-O2	6.88	123.03	118.90
1	2A	2136	C	C2-N3-C4	6.81	123.31	119.90
54	2w	21	A	N9-C4-C5	6.75	108.50	105.80
1	2A	2155	G	C6-N1-C2	6.74	129.15	125.10
1	2A	2492	U	O5'-P-OP1	-6.67	99.69	105.70
55	1x	14	A	C5-C6-N1	-6.62	114.39	117.70
1	1A	1190	G	C5-N7-C8	6.60	107.60	104.30
1	1A	2134	A	P-O3'-C3'	6.60	127.61	119.70
32	2a	754	C	N1-C2-O2	6.54	122.82	118.90
1	2A	1313	U	C2-N1-C1'	6.45	125.44	117.70
32	1a	266	G	P-O3'-C3'	6.42	127.41	119.70
56	2y	25	C	C2-N1-C1'	6.38	125.82	118.80
1	2A	2136	C	N3-C2-O2	-6.37	117.44	121.90
1	1A	2848	G	O4'-C1'-N9	6.35	113.28	108.20
32	1a	1034	G	C6-N1-C2	6.34	128.90	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1263	C	C6-N1-C2	-6.31	117.78	120.30
55	1x	22	G	C5-C6-N1	6.27	114.64	111.50
55	1x	46	G	C5-C6-N1	6.27	114.63	111.50
56	2y	33	U	N3-C2-O2	-6.23	117.84	122.20
32	2a	841	U	C5-C6-N1	6.21	125.81	122.70
32	2a	1138	G	C4-N9-C1'	6.20	134.56	126.50
55	1x	22	G	N1-C6-O6	-6.20	116.18	119.90
32	1a	254	G	O5'-P-OP1	-6.19	100.13	105.70
1	1A	2790	A	C2-N3-C4	6.14	113.67	110.60
1	2A	1204	A	O4'-C1'-N9	6.10	113.08	108.20
1	1A	2554	U	O5'-P-OP1	-6.10	100.21	105.70
1	1A	2629	A	P-O3'-C3'	6.10	127.02	119.70
1	2A	512	G	O4'-C1'-N9	6.09	113.07	108.20
1	1A	372	G	O4'-C1'-N9	6.08	113.07	108.20
1	1A	1075	C	N3-C2-O2	-6.08	117.64	121.90
55	2x	22	G	C5-N7-C8	-6.07	101.26	104.30
56	2y	48	C	P-O3'-C3'	6.06	126.97	119.70
55	2x	46	G	N3-C2-N2	-6.05	115.67	119.90
1	1A	2167	U	C2-N1-C1'	6.05	124.96	117.70
1	1A	2502	G	O5'-P-OP2	-6.04	100.27	105.70
1	1A	1176	G	OP1-P-O3'	6.03	118.47	105.20
1	1A	847	U	C2-N1-C1'	6.02	124.92	117.70
32	2a	1263	C	N1-C2-N3	-6.01	114.99	119.20
32	2a	1263	C	C4-C5-C6	-6.01	114.40	117.40
55	1x	22	G	C4-C5-C6	-6.00	115.20	118.80
54	2w	14	A	C4-C5-N7	5.92	113.66	110.70
56	1y	69	C	C2-N1-C1'	5.92	125.31	118.80
1	2A	1022	G	N3-C4-N9	-5.89	122.47	126.00
1	1A	2430	A	O5'-P-OP2	-5.88	100.40	105.70
32	1a	1030(B)	C	C6-N1-C1'	-5.88	113.74	120.80
56	2y	14	A	N1-C6-N6	5.88	122.12	118.60
32	2a	266	G	P-O3'-C3'	5.85	126.72	119.70
55	1x	14	A	C8-N9-C1'	-5.84	117.19	127.70
56	2y	14	A	C5-C6-N6	-5.84	119.03	123.70
1	2A	1992	G	P-O3'-C3'	5.83	126.69	119.70
32	1a	1067	A	P-O3'-C3'	5.80	126.66	119.70
32	2a	1029	C	N1-C2-O2	5.79	122.37	118.90
1	1A	2167	U	N1-C2-O2	5.78	126.85	122.80
1	1A	1131	G	O4'-C1'-N9	5.78	112.82	108.20
1	1A	1313	U	C2-N1-C1'	5.76	124.61	117.70
54	2w	14	A	C5-C6-N1	5.76	120.58	117.70
1	1A	1992	G	P-O3'-C3'	5.74	126.59	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	2y	25	C	N1-C2-O2	5.73	122.34	118.90
1	1A	195	A	P-O3'-C3'	5.71	126.55	119.70
32	1a	1030(B)	C	C5-C6-N1	5.71	123.85	121.00
32	1a	841	U	C5-C6-N1	5.70	125.55	122.70
1	1A	2371	G	C5-C6-N1	5.69	114.35	111.50
1	1A	2682	U	O5'-P-OP2	-5.68	100.59	105.70
54	2w	14	A	C5-N7-C8	-5.67	101.07	103.90
1	1A	819	A	O5'-P-OP1	-5.67	100.60	105.70
54	1w	5	G	C8-N9-C1'	5.66	134.36	127.00
1	2A	2061	G	O5'-P-OP2	-5.65	100.61	105.70
55	2x	22	G	C4-C5-C6	-5.64	115.42	118.80
55	1x	14	A	C4-N9-C1'	5.64	136.44	126.30
1	1A	845	G	O4'-C1'-N9	5.63	112.70	108.20
1	1A	1352	U	O5'-P-OP1	-5.63	100.63	105.70
32	2a	1263	C	C5-C4-N4	5.63	124.14	120.20
54	1w	5	G	C6-C5-N7	5.62	133.77	130.40
1	1A	1063	G	C6-N1-C2	5.60	128.46	125.10
1	1A	2500	U	O4'-C1'-N1	5.59	112.68	108.20
56	2y	25	C	C6-N1-C1'	-5.59	114.09	120.80
1	1A	250	G	C8-N9-C4	-5.58	104.17	106.40
32	2a	1138	G	C8-N9-C1'	-5.58	119.75	127.00
1	2A	885	C	C5-C6-N1	5.56	123.78	121.00
1	1A	1174	A	P-O3'-C3'	5.55	126.36	119.70
54	1w	5	G	N3-C4-N9	-5.53	122.69	126.00
1	1A	805	G	N9-C4-C5	-5.51	103.19	105.40
1	2A	847	U	C2-N1-C1'	5.51	124.31	117.70
32	1a	1201	A	P-O3'-C3'	5.51	126.31	119.70
56	2y	72	C	N1-C2-O2	5.51	122.20	118.90
1	2A	1614	A	O5'-P-OP1	-5.50	100.75	105.70
1	1A	746	A	O4'-C1'-N9	5.49	112.59	108.20
1	2A	576	U	O5'-P-OP1	-5.48	100.77	105.70
32	2a	1225	A	N1-C6-N6	-5.47	115.32	118.60
54	1w	5	G	C4-N9-C1'	-5.46	119.40	126.50
1	2A	752	A	P-O3'-C3'	5.46	126.26	119.70
32	1a	792	A	O4'-C1'-N9	5.43	112.54	108.20
1	1A	1325	G	N9-C4-C5	5.43	107.57	105.40
54	1w	5	G	N9-C4-C5	5.42	107.57	105.40
1	2A	383	U	O4'-C1'-N1	5.42	112.53	108.20
1	1A	198	C	O5'-P-OP2	-5.42	100.82	105.70
1	1A	2059	A	O4'-C1'-N9	5.40	112.52	108.20
1	1A	548	A	P-O3'-C3'	5.40	126.18	119.70
32	1a	90	U	C2-N1-C1'	5.40	124.18	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1158	C	C2-N1-C1'	5.38	124.71	118.80
1	1A	847	U	N1-C2-O2	5.37	126.56	122.80
1	1A	975	C	C2-N3-C4	-5.35	117.23	119.90
32	1a	90	U	N3-C2-O2	-5.34	118.46	122.20
32	2a	1272	G	N3-C4-N9	5.33	129.20	126.00
56	2y	69	C	C2-N3-C4	5.33	122.56	119.90
54	2w	14	A	C6-N1-C2	-5.32	115.41	118.60
1	2A	1313	U	O4'-C1'-N1	5.32	112.46	108.20
1	2A	2712	U	O4'-C1'-N1	5.31	112.45	108.20
1	1A	774	A	C8-N9-C4	-5.31	103.68	105.80
54	1w	5	G	C4-C5-N7	-5.30	108.68	110.80
55	2x	14	A	C5-C6-N1	-5.30	115.05	117.70
1	1A	2282	G	O4'-C1'-N9	5.29	112.43	108.20
1	1A	1063	G	N3-C2-N2	5.29	123.60	119.90
1	2A	228	A	P-O3'-C3'	5.28	126.03	119.70
1	1A	1190	G	C4-C5-N7	-5.27	108.69	110.80
1	1A	1325	G	O4'-C1'-N9	5.26	112.40	108.20
32	1a	687	A	P-O3'-C3'	5.26	126.01	119.70
32	2a	1225	A	C5-C6-N6	5.25	127.90	123.70
1	1A	568	U	C5-C4-O4	-5.24	122.75	125.90
1	1A	2685	G	N1-C6-O6	-5.23	116.76	119.90
1	1A	2134	A	OP1-P-O3'	5.23	116.71	105.20
1	1A	72	U	O5'-P-OP1	-5.22	101.00	105.70
1	2A	1774	C	O5'-P-OP1	-5.22	101.00	105.70
1	2A	528	A	OP1-P-O3'	5.22	116.68	105.20
55	1x	46	G	C5-C6-O6	-5.20	125.48	128.60
1	1A	383	U	C2-N1-C1'	-5.19	111.47	117.70
32	2a	913	A	P-O3'-C3'	5.18	125.92	119.70
32	2a	1065	U	P-O3'-C3'	5.18	125.92	119.70
1	1A	954	G	O5'-P-OP1	-5.15	101.06	105.70
1	1A	271(Y)	U	O4'-C1'-N1	5.15	112.32	108.20
56	2y	68	C	N1-C2-O2	5.14	121.99	118.90
32	2a	687	A	P-O3'-C3'	5.13	125.86	119.70
32	1a	1531	A	N7-C8-N9	5.13	116.37	113.80
55	1x	46	G	N1-C2-N3	5.13	126.98	123.90
1	1A	568	U	N3-C4-C5	5.13	117.68	114.60
32	2a	754	C	C6-N1-C1'	-5.13	114.65	120.80
56	2y	70	C	C2-N1-C1'	5.12	124.43	118.80
1	1A	383	U	O4'-C1'-N1	5.11	112.29	108.20
32	1a	913	A	P-O3'-C3'	5.11	125.83	119.70
1	2A	2689	U	P-O3'-C3'	5.10	125.82	119.70
1	1A	1936	A	O4'-C1'-N9	5.09	112.27	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	560	U	C3'-C2'-C1'	5.08	105.56	101.50
1	1A	1164	G	N1-C6-O6	-5.07	116.86	119.90
1	1A	575	A	O5'-P-OP1	-5.06	101.15	105.70
1	1A	975	C	C2-N1-C1'	-5.05	113.24	118.80
32	1a	1206	G	N3-C4-N9	5.05	129.03	126.00
55	2x	22	G	C5-C6-N1	5.05	114.03	111.50
32	2a	754	C	N3-C2-O2	-5.05	118.36	121.90
1	1A	999	U	O5'-P-OP2	-5.05	101.15	105.70
1	1A	2167	U	N3-C2-O2	-5.04	118.67	122.20
1	1A	2789	C	N1-C2-O2	-5.04	115.88	118.90
32	1a	90	U	N1-C2-O2	5.03	126.32	122.80
1	2A	1131	G	O4'-C1'-N9	5.03	112.22	108.20
55	2x	46	G	C5-C6-N1	5.02	114.01	111.50
1	1A	1086	A	N1-C6-N6	-5.02	115.59	118.60
54	2w	21	A	N3-C4-N9	-5.01	123.39	127.40
55	1x	22	G	N7-C8-N9	5.00	115.60	113.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	1P	35	HIS	Peptide
11	2P	35	HIS	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%)	258 (94%)	15 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	2D	273/276 (99%)	256 (94%)	17 (6%)	0	100	100
4	1E	202/206 (98%)	190 (94%)	11 (5%)	1 (0%)	29	40
4	2E	202/206 (98%)	192 (95%)	9 (4%)	1 (0%)	29	40
5	1F	200/210 (95%)	194 (97%)	5 (2%)	1 (0%)	29	40
5	2F	200/210 (95%)	188 (94%)	10 (5%)	2 (1%)	15	22
6	1G	179/182 (98%)	161 (90%)	16 (9%)	2 (1%)	14	19
6	2G	179/182 (98%)	157 (88%)	19 (11%)	3 (2%)	9	11
7	1H	172/180 (96%)	160 (93%)	11 (6%)	1 (1%)	25	34
7	2H	172/180 (96%)	157 (91%)	14 (8%)	1 (1%)	25	34
8	1I	144/148 (97%)	129 (90%)	15 (10%)	0	100	100
8	2I	144/148 (97%)	126 (88%)	17 (12%)	1 (1%)	22	30
9	1N	138/140 (99%)	130 (94%)	7 (5%)	1 (1%)	22	30
9	2N	138/140 (99%)	129 (94%)	8 (6%)	1 (1%)	22	30
10	1O	120/122 (98%)	113 (94%)	6 (5%)	1 (1%)	19	27
10	2O	120/122 (98%)	115 (96%)	4 (3%)	1 (1%)	19	27
11	1P	147/150 (98%)	136 (92%)	9 (6%)	2 (1%)	11	15
11	2P	147/150 (98%)	132 (90%)	13 (9%)	2 (1%)	11	15
12	1Q	139/141 (99%)	132 (95%)	7 (5%)	0	100	100
12	2Q	139/141 (99%)	131 (94%)	8 (6%)	0	100	100
13	1R	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
13	2R	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
14	1S	108/112 (96%)	104 (96%)	4 (4%)	0	100	100
14	2S	108/112 (96%)	100 (93%)	7 (6%)	1 (1%)	17	24
15	1T	129/146 (88%)	120 (93%)	7 (5%)	2 (2%)	9	12
15	2T	129/146 (88%)	124 (96%)	5 (4%)	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%)	94 (95%)	4 (4%)	1 (1%)	15	22
17	2V	99/101 (98%)	93 (94%)	5 (5%)	1 (1%)	15	22
18	1W	110/113 (97%)	110 (100%)	0	0	100	100
18	2W	110/113 (97%)	108 (98%)	1 (1%)	1 (1%)	17	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	1X	93/96 (97%)	89 (96%)	2 (2%)	2 (2%)	6	7
19	2X	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
20	1Y	105/110 (96%)	97 (92%)	6 (6%)	2 (2%)	8	9
20	2Y	105/110 (96%)	95 (90%)	7 (7%)	3 (3%)	4	4
21	1Z	148/206 (72%)	127 (86%)	19 (13%)	2 (1%)	11	15
21	2Z	156/206 (76%)	132 (85%)	22 (14%)	2 (1%)	12	16
22	10	81/85 (95%)	80 (99%)	1 (1%)	0	100	100
22	20	81/85 (95%)	79 (98%)	2 (2%)	0	100	100
23	11	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	14	19
23	21	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	14	19
24	12	68/72 (94%)	65 (96%)	3 (4%)	0	100	100
24	22	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
25	13	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
25	23	57/60 (95%)	54 (95%)	2 (4%)	1 (2%)	8	10
26	14	67/71 (94%)	53 (79%)	9 (13%)	5 (8%)	1	0
26	24	67/71 (94%)	49 (73%)	13 (19%)	5 (8%)	1	0
27	15	57/60 (95%)	57 (100%)	0	0	100	100
27	25	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
28	16	51/54 (94%)	51 (100%)	0	0	100	100
28	26	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
29	17	46/49 (94%)	45 (98%)	1 (2%)	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%)	62 (100%)	0	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
33	1b	229/256 (90%)	192 (84%)	30 (13%)	7 (3%)	4	3
33	2b	229/256 (90%)	181 (79%)	43 (19%)	5 (2%)	6	7
34	1c	204/239 (85%)	184 (90%)	20 (10%)	0	100	100
34	2c	204/239 (85%)	173 (85%)	29 (14%)	2 (1%)	15	22
35	1d	206/209 (99%)	188 (91%)	17 (8%)	1 (0%)	29	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	2d	206/209 (99%)	186 (90%)	20 (10%)	0	100	100
36	1e	146/162 (90%)	132 (90%)	13 (9%)	1 (1%)	22	30
36	2e	146/162 (90%)	130 (89%)	15 (10%)	1 (1%)	22	30
37	1f	98/101 (97%)	94 (96%)	3 (3%)	1 (1%)	15	22
37	2f	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
38	1g	153/156 (98%)	142 (93%)	9 (6%)	2 (1%)	12	16
38	2g	153/156 (98%)	136 (89%)	14 (9%)	3 (2%)	7	8
39	1h	135/138 (98%)	127 (94%)	8 (6%)	0	100	100
39	2h	135/138 (98%)	125 (93%)	9 (7%)	1 (1%)	22	30
40	1i	125/128 (98%)	114 (91%)	10 (8%)	1 (1%)	19	27
40	2i	125/128 (98%)	102 (82%)	23 (18%)	0	100	100
41	1j	95/105 (90%)	83 (87%)	8 (8%)	4 (4%)	3	1
41	2j	94/105 (90%)	80 (85%)	10 (11%)	4 (4%)	2	1
42	1k	112/129 (87%)	101 (90%)	8 (7%)	3 (3%)	5	4
42	2k	112/129 (87%)	98 (88%)	13 (12%)	1 (1%)	17	24
43	1l	119/132 (90%)	114 (96%)	4 (3%)	1 (1%)	19	27
43	2l	119/132 (90%)	109 (92%)	9 (8%)	1 (1%)	19	27
44	1m	121/126 (96%)	107 (88%)	12 (10%)	2 (2%)	9	11
44	2m	120/126 (95%)	99 (82%)	18 (15%)	3 (2%)	5	5
45	1n	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
45	2n	58/61 (95%)	54 (93%)	4 (7%)	0	100	100
46	1o	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
46	2o	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
47	1p	80/88 (91%)	70 (88%)	9 (11%)	1 (1%)	12	16
47	2p	80/88 (91%)	70 (88%)	10 (12%)	0	100	100
48	1q	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
48	2q	97/105 (92%)	88 (91%)	7 (7%)	2 (2%)	7	7
49	1r	66/88 (75%)	62 (94%)	4 (6%)	0	100	100
49	2r	66/88 (75%)	64 (97%)	1 (2%)	1 (2%)	10	14
50	1s	81/93 (87%)	70 (86%)	10 (12%)	1 (1%)	13	17
50	2s	81/93 (87%)	64 (79%)	15 (18%)	2 (2%)	5	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	1t	94/106 (89%)	86 (92%)	5 (5%)	3 (3%)	4	3
51	2t	94/106 (89%)	83 (88%)	10 (11%)	1 (1%)	14	19
52	1u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
52	2u	21/27 (78%)	18 (86%)	3 (14%)	0	100	100
All	All	11368/12128 (94%)	10449 (92%)	813 (7%)	106 (1%)	17	24

All (106) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
21	1Z	53	ILE
26	14	47	GLN
26	14	49	PHE
26	14	62	ARG
33	1b	17	PHE
40	1i	54	ASP
44	1m	67	GLU
5	2F	130	ALA
6	2G	124	SER
33	2b	123	ALA
38	2g	80	VAL
44	2m	67	GLU
50	2s	12	ASP
6	1G	43	LEU
15	1T	37	GLY
19	1X	93	GLU
23	11	3	LYS
33	1b	8	LYS
33	1b	126	GLU
36	1e	85	GLY
41	1j	79	ARG
42	1k	77	MET
42	1k	105	VAL
8	2I	10	GLU
17	2V	79	VAL
20	2Y	55	TYR
26	24	3	GLU
26	24	45	GLY
33	2b	17	PHE
33	2b	20	GLU
34	2c	91	LEU

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Mol	Chain	Res	Type
36	2e	85	GLY
38	2g	55	GLY
42	2k	49	GLY
49	2r	36	ASN
6	1G	96	ARG
17	1V	79	VAL
21	1Z	52	SER
33	1b	124	SER
5	2F	18	ARG
6	2G	51	ARG
7	2H	126	PRO
9	2N	2	LYS
11	2P	44	GLY
11	2P	45	LEU
26	24	48	ARG
33	2b	9	GLU
33	2b	10	LEU
41	2j	79	ARG
44	2m	106	ASN
48	2q	33	GLY
4	1E	52	LEU
9	1N	2	LYS
11	1P	29	LYS
11	1P	38	GLN
20	1Y	54	LYS
20	1Y	103	GLY
26	14	57	GLU
38	1g	114	ARG
41	1j	78	ASN
43	1l	105	TYR
51	1t	100	ILE
4	2E	52	LEU
6	2G	43	LEU
23	2l	3	LYS
34	2c	156	ARG
43	2l	105	TYR
44	2m	63	THR
50	2s	81	ARG
7	1H	126	PRO
10	1O	5	GLN
15	1T	128	GLU
19	1X	2	LYS

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Mol	Chain	Res	Type
33	1b	19	HIS
35	1d	175	SER
41	1j	29	ARG
44	1m	106	ASN
47	1p	76	GLN
51	1t	47	GLY
51	1t	95	ALA
10	2O	5	GLN
14	2S	96	GLY
18	2W	60	ASN
20	2Y	54	LYS
21	2Z	146	ILE
26	24	49	PHE
38	2g	52	GLU
41	2j	75	ILE
41	2j	78	ASN
48	2q	68	ARG
38	1g	54	THR
50	1s	27	GLU
20	2Y	11	ASP
21	2Z	52	SER
26	14	45	GLY
25	23	59	VAL
41	2j	41	PRO
33	1b	231	GLU
42	1k	49	GLY
37	1f	40	VAL
26	24	11	PRO
51	2t	47	GLY
41	1j	77	PRO
39	2h	86	ILE
33	1b	125	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	215/218 (99%)	203 (94%)	12 (6%)	21	28
3	2D	215/218 (99%)	204 (95%)	11 (5%)	24	32
4	1E	164/166 (99%)	157 (96%)	7 (4%)	29	39
4	2E	164/166 (99%)	157 (96%)	7 (4%)	29	39
5	1F	160/166 (96%)	144 (90%)	16 (10%)	7	8
5	2F	159/166 (96%)	153 (96%)	6 (4%)	33	45
6	1G	143/156 (92%)	131 (92%)	12 (8%)	11	13
6	2G	143/156 (92%)	126 (88%)	17 (12%)	5	5
7	1H	144/148 (97%)	139 (96%)	5 (4%)	36	49
7	2H	144/148 (97%)	134 (93%)	10 (7%)	15	20
8	1I	113/124 (91%)	96 (85%)	17 (15%)	3	2
8	2I	105/124 (85%)	94 (90%)	11 (10%)	7	7
9	1N	118/119 (99%)	114 (97%)	4 (3%)	37	50
9	2N	118/119 (99%)	111 (94%)	7 (6%)	19	25
10	1O	100/100 (100%)	98 (98%)	2 (2%)	55	70
10	2O	100/100 (100%)	98 (98%)	2 (2%)	55	70
11	1P	115/116 (99%)	107 (93%)	8 (7%)	15	19
11	2P	115/116 (99%)	106 (92%)	9 (8%)	12	16
12	1Q	111/111 (100%)	107 (96%)	4 (4%)	35	47
12	2Q	111/111 (100%)	106 (96%)	5 (4%)	27	37
13	1R	101/101 (100%)	95 (94%)	6 (6%)	19	25
13	2R	101/101 (100%)	98 (97%)	3 (3%)	41	55
14	1S	86/88 (98%)	79 (92%)	7 (8%)	11	14
14	2S	85/88 (97%)	77 (91%)	8 (9%)	8	10
15	1T	115/127 (91%)	110 (96%)	5 (4%)	29	39
15	2T	113/127 (89%)	107 (95%)	6 (5%)	22	30
16	1U	93/94 (99%)	90 (97%)	3 (3%)	39	53
16	2U	93/94 (99%)	89 (96%)	4 (4%)	29	39
17	1V	80/82 (98%)	78 (98%)	2 (2%)	47	62
17	2V	80/82 (98%)	75 (94%)	5 (6%)	18	23
18	1W	90/92 (98%)	86 (96%)	4 (4%)	28	38
18	2W	90/92 (98%)	85 (94%)	5 (6%)	21	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	1X	77/78 (99%)	76 (99%)	1 (1%)	69	80
19	2X	77/78 (99%)	75 (97%)	2 (3%)	46	61
20	1Y	85/91 (93%)	82 (96%)	3 (4%)	36	49
20	2Y	85/91 (93%)	78 (92%)	7 (8%)	11	14
21	1Z	135/179 (75%)	124 (92%)	11 (8%)	11	14
21	2Z	137/179 (76%)	124 (90%)	13 (10%)	8	10
22	10	65/67 (97%)	64 (98%)	1 (2%)	65	77
22	20	65/67 (97%)	63 (97%)	2 (3%)	40	54
23	11	80/83 (96%)	79 (99%)	1 (1%)	69	80
23	21	80/83 (96%)	74 (92%)	6 (8%)	13	17
24	12	65/67 (97%)	64 (98%)	1 (2%)	65	77
24	22	65/67 (97%)	63 (97%)	2 (3%)	40	54
25	13	51/52 (98%)	46 (90%)	5 (10%)	8	9
25	23	50/52 (96%)	48 (96%)	2 (4%)	31	43
26	14	59/63 (94%)	51 (86%)	8 (14%)	3	3
26	24	53/63 (84%)	42 (79%)	11 (21%)	1	1
27	15	50/52 (96%)	48 (96%)	2 (4%)	31	43
27	25	50/52 (96%)	46 (92%)	4 (8%)	12	15
28	16	51/52 (98%)	49 (96%)	2 (4%)	32	44
28	26	50/52 (96%)	46 (92%)	4 (8%)	12	15
29	17	41/42 (98%)	37 (90%)	4 (10%)	8	9
29	27	41/42 (98%)	37 (90%)	4 (10%)	8	9
30	18	54/55 (98%)	51 (94%)	3 (6%)	21	28
30	28	54/55 (98%)	50 (93%)	4 (7%)	13	18
31	19	34/34 (100%)	34 (100%)	0	100	100
31	29	34/34 (100%)	31 (91%)	3 (9%)	10	12
33	1b	192/220 (87%)	172 (90%)	20 (10%)	7	7
33	2b	187/220 (85%)	161 (86%)	26 (14%)	3	3
34	1c	142/188 (76%)	130 (92%)	12 (8%)	10	13
34	2c	140/188 (74%)	128 (91%)	12 (9%)	10	13
35	1d	169/181 (93%)	150 (89%)	19 (11%)	6	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	2d	173/181 (96%)	152 (88%)	21 (12%)	5	4
36	1e	113/123 (92%)	106 (94%)	7 (6%)	18	24
36	2e	114/123 (93%)	102 (90%)	12 (10%)	7	7
37	1f	84/90 (93%)	81 (96%)	3 (4%)	35	47
37	2f	85/90 (94%)	80 (94%)	5 (6%)	19	25
38	1g	119/127 (94%)	104 (87%)	15 (13%)	4	4
38	2g	120/127 (94%)	112 (93%)	8 (7%)	16	21
39	1h	114/119 (96%)	108 (95%)	6 (5%)	22	30
39	2h	114/119 (96%)	106 (93%)	8 (7%)	15	19
40	1i	90/99 (91%)	79 (88%)	11 (12%)	5	4
40	2i	89/99 (90%)	79 (89%)	10 (11%)	6	5
41	1j	66/92 (72%)	58 (88%)	8 (12%)	5	4
41	2j	69/92 (75%)	61 (88%)	8 (12%)	5	5
42	1k	82/99 (83%)	76 (93%)	6 (7%)	14	18
42	2k	83/99 (84%)	77 (93%)	6 (7%)	14	18
43	1l	96/108 (89%)	90 (94%)	6 (6%)	18	23
43	2l	96/108 (89%)	88 (92%)	8 (8%)	11	14
44	1m	93/101 (92%)	85 (91%)	8 (9%)	10	13
44	2m	92/101 (91%)	88 (96%)	4 (4%)	29	39
45	1n	49/50 (98%)	43 (88%)	6 (12%)	5	4
45	2n	49/50 (98%)	43 (88%)	6 (12%)	5	4
46	1o	78/80 (98%)	74 (95%)	4 (5%)	24	32
46	2o	78/80 (98%)	75 (96%)	3 (4%)	33	45
47	1p	69/74 (93%)	62 (90%)	7 (10%)	7	8
47	2p	68/74 (92%)	63 (93%)	5 (7%)	13	18
48	1q	94/97 (97%)	90 (96%)	4 (4%)	29	39
48	2q	94/97 (97%)	88 (94%)	6 (6%)	17	23
49	1r	59/77 (77%)	58 (98%)	1 (2%)	60	75
49	2r	59/77 (77%)	56 (95%)	3 (5%)	24	32
50	1s	69/80 (86%)	67 (97%)	2 (3%)	42	57
50	2s	67/80 (84%)	57 (85%)	10 (15%)	3	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	1t	70/82 (85%)	66 (94%)	4 (6%)	20	27
51	2t	70/82 (85%)	66 (94%)	4 (6%)	20	27
52	1u	18/22 (82%)	18 (100%)	0	100	100
52	2u	18/22 (82%)	17 (94%)	1 (6%)	21	28
All	All	9303/10064 (92%)	8652 (93%)	651 (7%)	15	19

All (651) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	3	VAL
3	1D	14	ARG
3	1D	16	MET
3	1D	38	LYS
3	1D	99	ASP
3	1D	155	LEU
3	1D	211	ARG
3	1D	229	VAL
3	1D	242	ARG
3	1D	259	THR
3	1D	273	ARG
3	1D	275	LYS
4	1E	21	VAL
4	1E	73	GLU
4	1E	113	PHE
4	1E	116	VAL
4	1E	128	SER
4	1E	181	LEU
4	1E	184	VAL
5	1F	24	LEU
5	1F	28	ILE
5	1F	53	THR
5	1F	57	VAL
5	1F	60	SER
5	1F	70	THR
5	1F	74	ARG
5	1F	88	VAL
5	1F	106	ARG
5	1F	144	LYS
5	1F	162	LEU
5	1F	168	ARG
5	1F	175	THR

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Mol	Chain	Res	Type
5	1F	183	VAL
5	1F	192	LEU
5	1F	205	ARG
6	1G	3	LEU
6	1G	4	ASP
6	1G	7	LEU
6	1G	31	VAL
6	1G	43	LEU
6	1G	49	ASP
6	1G	79	ASN
6	1G	126	ASP
6	1G	133	LEU
6	1G	146	TYR
6	1G	148	MET
6	1G	159	VAL
7	1H	3	ARG
7	1H	30	LYS
7	1H	127	GLU
7	1H	152	ARG
7	1H	155	SER
8	1I	10	GLU
8	1I	20	ASP
8	1I	38	LEU
8	1I	47	LEU
8	1I	75	LEU
8	1I	76	THR
8	1I	77	LEU
8	1I	78	THR
8	1I	85	GLU
8	1I	87	LYS
8	1I	92	VAL
8	1I	108	THR
8	1I	109	ILE
8	1I	116	LEU
8	1I	127	VAL
8	1I	133	HIS
8	1I	142	VAL
9	1N	1	MET
9	1N	14	VAL
9	1N	28	THR
9	1N	48	MET
10	1O	28	SER

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Mol	Chain	Res	Type
10	1O	113	LYS
11	1P	7	ARG
11	1P	45	LEU
11	1P	56	SER
11	1P	65	ARG
11	1P	90	ARG
11	1P	96	THR
11	1P	135	LEU
11	1P	147	LEU
12	1Q	6	ARG
12	1Q	7	MET
12	1Q	56	ARG
12	1Q	75	THR
13	1R	36	THR
13	1R	59	ASP
13	1R	67	LEU
13	1R	104	ARG
13	1R	111	LEU
13	1R	114	VAL
14	1S	25	ARG
14	1S	36	TYR
14	1S	46	VAL
14	1S	69	VAL
14	1S	73	LEU
14	1S	85	VAL
14	1S	110	LEU
15	1T	28	VAL
15	1T	36	GLU
15	1T	49	VAL
15	1T	67	SER
15	1T	128	GLU
16	1U	19	LYS
16	1U	74	LEU
16	1U	77	SER
17	1V	61	VAL
17	1V	79	VAL
18	1W	11	ARG
18	1W	17	VAL
18	1W	63	ASP
18	1W	67	ASP
19	1X	68	ARG
20	1Y	23	ARG

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Mol	Chain	Res	Type
20	1Y	99	CYS
20	1Y	106	LEU
21	1Z	46	LYS
21	1Z	49	ARG
21	1Z	50	GLN
21	1Z	61	LEU
21	1Z	66	SER
21	1Z	128	VAL
21	1Z	132	ASN
21	1Z	154	ASP
21	1Z	155	LEU
21	1Z	170	THR
21	1Z	171	ILE
22	10	55	ARG
23	11	65	SER
24	12	40	SER
25	13	23	LEU
25	13	44	ARG
25	13	54	VAL
25	13	55	ARG
25	13	60	GLU
26	14	5	ILE
26	14	49	PHE
26	14	52	THR
26	14	53	GLU
26	14	59	PHE
26	14	60	GLN
26	14	63	TYR
26	14	67	TYR
27	15	6	VAL
27	15	40	LYS
28	16	4	GLU
28	16	19	ARG
29	17	24	THR
29	17	41	ARG
29	17	43	THR
29	17	46	VAL
30	18	29	LYS
30	18	31	HIS
30	18	34	TRP
33	1b	8	LYS
33	1b	11	LEU

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Mol	Chain	Res	Type
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	45	GLN
33	1b	54	THR
33	1b	60	ASP
33	1b	64	ARG
33	1b	67	THR
33	1b	76	GLN
33	1b	80	ILE
33	1b	112	VAL
33	1b	147	LYS
33	1b	185	ILE
33	1b	212	GLN
33	1b	215	LEU
34	1c	3	ASN
34	1c	15	THR
34	1c	21	ARG
34	1c	26	LYS
34	1c	46	GLU
34	1c	89	GLU
34	1c	97	LYS
34	1c	105	GLU
34	1c	138	VAL
34	1c	188	LEU
34	1c	196	LEU
34	1c	198	VAL
35	1d	10	ARG
35	1d	19	LEU
35	1d	28	SER
35	1d	31	CYS
35	1d	53	ASP
35	1d	56	VAL
35	1d	59	ARG
35	1d	88	VAL
35	1d	112	VAL
35	1d	135	LEU
35	1d	141	ARG
35	1d	144	ASP

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Mol	Chain	Res	Type
35	1d	157	LEU
35	1d	175	SER
35	1d	177	ASP
35	1d	178	VAL
35	1d	181	MET
35	1d	188	LEU
35	1d	194	LEU
36	1e	10	MET
36	1e	20	GLN
36	1e	41	VAL
36	1e	51	VAL
36	1e	56	GLN
36	1e	63	ARG
36	1e	151	LEU
37	1f	36	ARG
37	1f	75	LEU
37	1f	77	ARG
38	1g	8	GLU
38	1g	12	LEU
38	1g	24	THR
38	1g	32	ARG
38	1g	50	ILE
38	1g	57	GLU
38	1g	61	VAL
38	1g	78	ARG
38	1g	97	GLN
38	1g	104	LEU
38	1g	113	GLU
38	1g	138	LYS
38	1g	140	ASP
38	1g	143	ARG
38	1g	156	TRP
39	1h	39	LEU
39	1h	52	ASP
39	1h	54	ASP
39	1h	68	ARG
39	1h	112	LEU
39	1h	122	ARG
40	1i	23	ASN
40	1i	25	LYS
40	1i	34	ASN
40	1i	50	LEU

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Mol	Chain	Res	Type
40	1i	53	VAL
40	1i	71	SER
40	1i	89	ASN
40	1i	96	LEU
40	1i	103	THR
40	1i	111	ARG
40	1i	128	ARG
41	1j	38	ILE
41	1j	42	THR
41	1j	48	THR
41	1j	49	VAL
41	1j	51	ARG
41	1j	81	THR
41	1j	94	VAL
41	1j	98	ILE
42	1k	14	VAL
42	1k	25	TYR
42	1k	33	THR
42	1k	48	ILE
42	1k	87	THR
42	1k	114	VAL
43	1l	18	VAL
43	1l	33	ARG
43	1l	36	VAL
43	1l	46	LYS
43	1l	116	SER
43	1l	123	LYS
44	1m	4	ILE
44	1m	43	THR
44	1m	49	THR
44	1m	70	LEU
44	1m	79	LYS
44	1m	106	ASN
44	1m	109	THR
44	1m	120	LYS
45	1n	15	LYS
45	1n	18	VAL
45	1n	29	ARG
45	1n	33	VAL
45	1n	41	ARG
45	1n	56	VAL
46	1o	39	LEU

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Mol	Chain	Res	Type
46	1o	56	LEU
46	1o	76	GLU
46	1o	84	LYS
47	1p	5	ARG
47	1p	19	ILE
47	1p	20	VAL
47	1p	42	ARG
47	1p	60	LEU
47	1p	62	VAL
47	1p	76	GLN
48	1q	45	HIS
48	1q	57	VAL
48	1q	66	SER
48	1q	79	SER
49	1r	46	GLU
50	1s	6	LYS
50	1s	12	ASP
51	1t	10	LEU
51	1t	24	LEU
51	1t	53	LEU
51	1t	100	ILE
3	2D	3	VAL
3	2D	38	LYS
3	2D	141	VAL
3	2D	155	LEU
3	2D	162	SER
3	2D	173	VAL
3	2D	211	ARG
3	2D	229	VAL
3	2D	242	ARG
3	2D	259	THR
3	2D	275	LYS
4	2E	7	VAL
4	2E	21	VAL
4	2E	73	GLU
4	2E	90	THR
4	2E	116	VAL
4	2E	178	GLU
4	2E	181	LEU
5	2F	33	LEU
5	2F	135	LYS
5	2F	158	THR

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Mol	Chain	Res	Type
5	2F	160	ASN
5	2F	186	ILE
5	2F	192	LEU
6	2G	5	VAL
6	2G	21	ARG
6	2G	28	VAL
6	2G	31	VAL
6	2G	47	LYS
6	2G	49	ASP
6	2G	79	ASN
6	2G	88	ILE
6	2G	91	ARG
6	2G	124	SER
6	2G	135	LEU
6	2G	137	GLU
6	2G	140	ILE
6	2G	148	MET
6	2G	149	VAL
6	2G	159	VAL
6	2G	170	ARG
7	2H	7	LEU
7	2H	15	VAL
7	2H	44	VAL
7	2H	45	VAL
7	2H	51	ARG
7	2H	85	LYS
7	2H	98	LEU
7	2H	130	ARG
7	2H	133	VAL
7	2H	152	ARG
8	2I	15	VAL
8	2I	20	ASP
8	2I	38	LEU
8	2I	40	THR
8	2I	61	ARG
8	2I	68	LEU
8	2I	69	LYS
8	2I	74	ASN
8	2I	81	VAL
8	2I	82	ARG
8	2I	117	GLU
9	2N	5	VAL

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Mol	Chain	Res	Type
9	2N	14	VAL
9	2N	15	LEU
9	2N	28	THR
9	2N	38	HIS
9	2N	67	LEU
9	2N	131	GLN
10	2O	9	GLU
10	2O	69	ILE
11	2P	7	ARG
11	2P	45	LEU
11	2P	65	ARG
11	2P	90	ARG
11	2P	96	THR
11	2P	131	SER
11	2P	133	SER
11	2P	135	LEU
11	2P	136	GLU
12	2Q	7	MET
12	2Q	12	GLN
12	2Q	75	THR
12	2Q	106	VAL
12	2Q	110	THR
13	2R	67	LEU
13	2R	111	LEU
13	2R	114	VAL
14	2S	35	ILE
14	2S	36	TYR
14	2S	44	LYS
14	2S	58	LEU
14	2S	63	THR
14	2S	83	LYS
14	2S	85	VAL
14	2S	110	LEU
15	2T	18	ASP
15	2T	28	VAL
15	2T	39	ARG
15	2T	85	LYS
15	2T	96	ARG
15	2T	104	ASN
16	2U	5	LYS
16	2U	65	ILE
16	2U	74	LEU

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Mol	Chain	Res	Type
16	2U	77	SER
17	2V	38	LEU
17	2V	56	SER
17	2V	61	VAL
17	2V	79	VAL
17	2V	85	LYS
18	2W	11	ARG
18	2W	15	ARG
18	2W	60	ASN
18	2W	63	ASP
18	2W	67	ASP
19	2X	60	ARG
19	2X	81	VAL
20	2Y	6	HIS
20	2Y	67	LEU
20	2Y	70	SER
20	2Y	72	VAL
20	2Y	85	VAL
20	2Y	98	VAL
20	2Y	99	CYS
21	2Z	5	LEU
21	2Z	42	VAL
21	2Z	66	SER
21	2Z	70	LEU
21	2Z	71	VAL
21	2Z	121	HIS
21	2Z	129	SER
21	2Z	150	LEU
21	2Z	154	ASP
21	2Z	155	LEU
21	2Z	161	VAL
21	2Z	171	ILE
21	2Z	174	VAL
22	20	10	THR
22	20	68	GLU
23	21	35	THR
23	21	40	ARG
23	21	46	LEU
23	21	56	GLN
23	21	81	LYS
23	21	83	GLU
24	22	35	LEU

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Mol	Chain	Res	Type
24	22	70	GLN
25	23	54	VAL
25	23	59	VAL
26	24	10	VAL
26	24	24	THR
26	24	29	PRO
26	24	33	VAL
26	24	34	GLU
26	24	49	PHE
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	40	LYS
27	25	58	LEU
28	26	6	ARG
28	26	19	ARG
28	26	29	ASN
28	26	48	VAL
29	27	1	MET
29	27	41	ARG
29	27	43	THR
29	27	46	VAL
30	28	14	VAL
30	28	29	LYS
30	28	31	HIS
30	28	34	TRP
31	29	6	SER
31	29	7	VAL
31	29	14	CYS
33	2b	7	VAL
33	2b	8	LYS
33	2b	16	HIS
33	2b	24	TRP
33	2b	55	PHE
33	2b	67	THR
33	2b	68	ILE
33	2b	71	VAL
33	2b	73	THR

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Mol	Chain	Res	Type
33	2b	76	GLN
33	2b	80	ILE
33	2b	101	MET
33	2b	107	THR
33	2b	112	VAL
33	2b	115	LEU
33	2b	118	LEU
33	2b	127	ILE
33	2b	138	LEU
33	2b	142	LEU
33	2b	185	ILE
33	2b	187	LEU
33	2b	189	ASP
33	2b	191	ASP
33	2b	220	ASP
33	2b	223	ILE
33	2b	233	SER
34	2c	15	THR
34	2c	35	GLU
34	2c	46	GLU
34	2c	47	LEU
34	2c	105	GLU
34	2c	111	LEU
34	2c	128	PHE
34	2c	153	VAL
34	2c	161	GLU
34	2c	173	VAL
34	2c	190	ARG
34	2c	191	THR
35	2d	5	ILE
35	2d	8	VAL
35	2d	12	CYS
35	2d	31	CYS
35	2d	34	GLU
35	2d	47	ARG
35	2d	53	ASP
35	2d	58	LEU
35	2d	59	ARG
35	2d	60	GLU
35	2d	76	ARG
35	2d	83	SER
35	2d	86	LYS

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Mol	Chain	Res	Type
35	2d	96	LEU
35	2d	123	HIS
35	2d	127	THR
35	2d	135	LEU
35	2d	150	GLU
35	2d	155	LEU
35	2d	156	GLU
35	2d	158	ILE
36	2e	5	ASP
36	2e	9	LYS
36	2e	13	ILE
36	2e	18	ARG
36	2e	20	GLN
36	2e	41	VAL
36	2e	51	VAL
36	2e	55	VAL
36	2e	73	ASN
36	2e	76	ILE
36	2e	78	HIS
36	2e	115	VAL
37	2f	21	LEU
37	2f	63	TYR
37	2f	69	GLU
37	2f	72	VAL
37	2f	81	ILE
38	2g	15	ASP
38	2g	52	GLU
38	2g	78	ARG
38	2g	79	ARG
38	2g	115	ARG
38	2g	131	LYS
38	2g	146	GLU
38	2g	155	ARG
39	2h	10	LEU
39	2h	26	VAL
39	2h	52	ASP
39	2h	54	ASP
39	2h	60	ARG
39	2h	77	GLU
39	2h	112	LEU
39	2h	113	SER
40	2i	32	ASP

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Mol	Chain	Res	Type
40	2i	54	ASP
40	2i	58	HIS
40	2i	65	VAL
40	2i	66	ARG
40	2i	99	LEU
40	2i	102	LEU
40	2i	108	VAL
40	2i	114	TYR
40	2i	128	ARG
41	2j	6	ILE
41	2j	9	ARG
41	2j	29	ARG
41	2j	38	ILE
41	2j	67	THR
41	2j	68	HIS
41	2j	69	ASN
41	2j	97	GLU
42	2k	41	THR
42	2k	48	ILE
42	2k	54	ARG
42	2k	105	VAL
42	2k	109	VAL
42	2k	117	ASN
43	2l	18	VAL
43	2l	33	ARG
43	2l	40	VAL
43	2l	53	ARG
43	2l	59	ARG
43	2l	62	SER
43	2l	112	ASP
43	2l	116	SER
44	2m	4	ILE
44	2m	62	ASN
44	2m	106	ASN
44	2m	110	ARG
45	2n	13	THR
45	2n	15	LYS
45	2n	18	VAL
45	2n	29	ARG
45	2n	41	ARG
45	2n	58	LYS
46	2o	39	LEU

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Mol	Chain	Res	Type
46	2o	76	GLU
46	2o	83	GLU
47	2p	1	MET
47	2p	2	VAL
47	2p	21	VAL
47	2p	73	LEU
47	2p	74	LEU
48	2q	5	VAL
48	2q	60	ILE
48	2q	63	ARG
48	2q	65	ILE
48	2q	66	SER
48	2q	99	SER
49	2r	28	GLU
49	2r	37	VAL
49	2r	85	LEU
50	2s	5	LEU
50	2s	12	ASP
50	2s	14	HIS
50	2s	16	LEU
50	2s	22	LEU
50	2s	27	GLU
50	2s	43	GLU
50	2s	45	VAL
50	2s	48	THR
50	2s	49	ILE
51	2t	9	ASN
51	2t	15	ARG
51	2t	46	GLU
51	2t	89	ARG
52	2u	9	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (113) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	87	ASN
5	1F	8	GLN
5	1F	69	HIS
6	1G	26	GLN
9	1N	131	GLN
12	1Q	12	GLN
13	1R	71	GLN

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Mol	Chain	Res	Type
14	1S	68	GLN
14	1S	95	HIS
15	1T	58	ASN
19	1X	31	HIS
19	1X	82	GLN
20	1Y	6	HIS
21	1Z	73	GLN
21	1Z	151	HIS
22	10	35	ASN
23	11	56	GLN
33	1b	40	HIS
33	1b	95	GLN
33	1b	212	GLN
34	1c	6	HIS
34	1c	118	GLN
34	1c	162	GLN
34	1c	176	HIS
35	1d	77	ASN
35	1d	116	GLN
35	1d	119	GLN
35	1d	123	HIS
36	1e	78	HIS
37	1f	18	GLN
37	1f	57	GLN
37	1f	100	ASN
38	1g	28	ASN
38	1g	51	GLN
40	1i	3	GLN
40	1i	31	GLN
40	1i	34	ASN
40	1i	58	HIS
40	1i	73	GLN
40	1i	89	ASN
40	1i	124	GLN
41	1j	56	HIS
43	1l	99	HIS
44	1m	77	ASN
46	1o	9	GLN
47	1p	13	HIS
48	1q	93	GLN
49	1r	63	GLN
50	1s	23	ASN

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Mol	Chain	Res	Type
50	1s	47	HIS
50	1s	83	HIS
51	1t	9	ASN
51	1t	90	GLN
3	2D	87	ASN
4	2E	48	GLN
5	2F	69	HIS
5	2F	160	ASN
6	2G	41	GLN
6	2G	58	GLN
6	2G	132	ASN
7	2H	74	ASN
8	2I	133	HIS
8	2I	139	GLN
9	2N	131	GLN
10	2O	5	GLN
12	2Q	12	GLN
13	2R	71	GLN
14	2S	38	GLN
15	2T	43	GLN
15	2T	58	ASN
15	2T	123	GLN
19	2X	31	HIS
19	2X	82	GLN
21	2Z	55	HIS
21	2Z	73	GLN
23	21	56	GLN
24	22	70	GLN
25	23	32	GLN
26	24	46	GLN
33	2b	76	GLN
33	2b	110	GLN
33	2b	135	GLN
33	2b	140	HIS
34	2c	6	HIS
34	2c	123	GLN
34	2c	162	GLN
35	2d	116	GLN
35	2d	119	GLN
35	2d	123	HIS
35	2d	161	ASN
36	2e	72	GLN

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Mol	Chain	Res	Type
37	2f	73	ASN
37	2f	100	ASN
38	2g	11	GLN
38	2g	28	ASN
38	2g	86	GLN
40	2i	3	GLN
40	2i	58	HIS
41	2j	13	HIS
41	2j	21	GLN
42	2k	62	GLN
42	2k	93	GLN
42	2k	104	GLN
42	2k	117	ASN
43	2l	99	HIS
44	2m	62	ASN
44	2m	77	ASN
48	2q	93	GLN
49	2r	63	GLN
50	2s	57	HIS
50	2s	69	HIS
50	2s	83	HIS
51	2t	75	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2863/2915 (98%)	414 (14%)	32 (1%)
1	2A	2790/2915 (95%)	430 (15%)	25 (0%)
2	1B	119/121 (98%)	7 (5%)	0
2	2B	118/121 (97%)	23 (19%)	0
32	1a	1494/1521 (98%)	231 (15%)	0
32	2a	1498/1521 (98%)	279 (18%)	0
53	1v	12/24 (50%)	2 (16%)	0
53	2v	12/24 (50%)	2 (16%)	0
54	1w	70/74 (94%)	27 (38%)	0
54	2w	68/74 (91%)	31 (45%)	0
55	1x	75/77 (97%)	7 (9%)	0
55	2x	75/77 (97%)	7 (9%)	0
56	1y	71/74 (95%)	29 (40%)	0
56	2y	71/74 (95%)	35 (49%)	0
All	All	9336/9612 (97%)	1524 (16%)	57 (0%)

All (1524) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	10	G
1	1A	12	U
1	1A	34	C
1	1A	45	C
1	1A	71	A
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	154(A)	C
1	1A	188	G
1	1A	196	A
1	1A	199	A
1	1A	205	G
1	1A	214	G
1	1A	215	G
1	1A	216	A
1	1A	221	A
1	1A	222	A
1	1A	225	A
1	1A	228	A
1	1A	229	A
1	1A	233	A
1	1A	248	G
1	1A	269	U
1	1A	271(A)	A
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	272(A)	U
1	1A	272(B)	G
1	1A	272(I)	U
1	1A	275	G
1	1A	279	C
1	1A	311	A
1	1A	329	G
1	1A	330	A

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Mol	Chain	Res	Type
1	1A	342	G
1	1A	352	G
1	1A	357	A
1	1A	363	G
1	1A	363(A)	A
1	1A	363(B)	G
1	1A	370	G
1	1A	386	G
1	1A	396	G
1	1A	405	U
1	1A	411	G
1	1A	412	A
1	1A	428	A
1	1A	444	C
1	1A	448	U
1	1A	451	C
1	1A	456	C
1	1A	457	A
1	1A	481	G
1	1A	494	G
1	1A	504	U
1	1A	505	A
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	568	U
1	1A	573	G
1	1A	574	C
1	1A	575	A
1	1A	586	A
1	1A	603	A
1	1A	604	G
1	1A	607	U
1	1A	614(A)	U
1	1A	614(B)	G
1	1A	615	G
1	1A	627	A

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Mol	Chain	Res	Type
1	1A	637	A
1	1A	645	C
1	1A	646	A
1	1A	652(D)	C
1	1A	652(E)	G
1	1A	652(F)	G
1	1A	652(T)	C
1	1A	669	G
1	1A	686	G
1	1A	730	C
1	1A	764	A
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	790	C
1	1A	792	G
1	1A	805	G
1	1A	812	C
1	1A	819	A
1	1A	827	U
1	1A	828	U
1	1A	859	G
1	1A	866	A
1	1A	877	U
1	1A	879	G
1	1A	880	G
1	1A	882	G
1	1A	883	G
1	1A	884	C
1	1A	885	C
1	1A	886	C
1	1A	887	A
1	1A	888	C
1	1A	889	C
1	1A	890	A
1	1A	895	U
1	1A	896	A
1	1A	897	C
1	1A	898	C

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Mol	Chain	Res	Type
1	1A	907	U
1	1A	910	A
1	1A	932	G
1	1A	938	G
1	1A	945	A
1	1A	946	G
1	1A	959	A
1	1A	961	C
1	1A	974	G
1	1A	975	C
1	1A	983	A
1	1A	996	A
1	1A	1012	U
1	1A	1013	C
1	1A	1026	U
1	1A	1033	U
1	1A	1041	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	1060	U
1	1A	1063	G
1	1A	1066	U
1	1A	1069	A
1	1A	1070	A
1	1A	1071	G
1	1A	1073	A
1	1A	1075	C
1	1A	1076	C
1	1A	1077	A
1	1A	1078	U
1	1A	1079	C
1	1A	1080	C
1	1A	1083	U
1	1A	1087	G
1	1A	1088	A
1	1A	1089	G
1	1A	1090	U
1	1A	1091	G

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Mol	Chain	Res	Type
1	1A	1093	G
1	1A	1094	U
1	1A	1096	A
1	1A	1097	U
1	1A	1101	U
1	1A	1110	G
1	1A	1111	A
1	1A	1112	G
1	1A	1116	C
1	1A	1135	C
1	1A	1136	G
1	1A	1141	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	1220	A
1	1A	1244	G
1	1A	1247	A
1	1A	1253	A
1	1A	1256	G
1	1A	1271	G
1	1A	1272	A
1	1A	1275	A
1	1A	1300	U
1	1A	1301	A
1	1A	1303	G
1	1A	1352	U
1	1A	1359	A
1	1A	1360	A
1	1A	1365	A
1	1A	1380	G
1	1A	1384	A
1	1A	1385	G
1	1A	1396	U
1	1A	1416	G
1	1A	1417	C
1	1A	1420	U
1	1A	1421	G

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Mol	Chain	Res	Type
1	1A	1428	C
1	1A	1445	A
1	1A	1450	G
1	1A	1455	G
1	1A	1467	C
1	1A	1482	G
1	1A	1493	C
1	1A	1494	A
1	1A	1508	A
1	1A	1509	C
1	1A	1509(A)	A
1	1A	1532	C
1	1A	1540	U
1	1A	1558	A
1	1A	1566	A
1	1A	1569	A
1	1A	1578	U
1	1A	1581	G
1	1A	1582	C
1	1A	1584	C
1	1A	1586	A
1	1A	1608	A
1	1A	1609	A
1	1A	1647	G
1	1A	1648	C
1	1A	1674	G
1	1A	1696	G
1	1A	1700	A
1	1A	1703	G
1	1A	1722	A
1	1A	1739	U
1	1A	1746	G
1	1A	1756	G
1	1A	1763	G
1	1A	1764	G
1	1A	1773	A
1	1A	1780	A
1	1A	1782	C
1	1A	1791	A
1	1A	1800	C
1	1A	1801	G
1	1A	1816	G

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Mol	Chain	Res	Type
1	1A	1828	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	1929	G
1	1A	1930	G
1	1A	1937	A
1	1A	1938	A
1	1A	1955	U
1	1A	1963	U
1	1A	1967	C
1	1A	1970	A
1	1A	1971	A
1	1A	1972	A
1	1A	1992	G
1	1A	1993	U
1	1A	1997	G
1	1A	2020	A
1	1A	2023	G
1	1A	2031	A
1	1A	2033	A
1	1A	2039	C
1	1A	2043	C
1	1A	2055	C
1	1A	2056	G
1	1A	2060	A
1	1A	2061	G
1	1A	2069	G
1	1A	2102	U
1	1A	2108	C
1	1A	2113	U
1	1A	2116	G
1	1A	2118	U
1	1A	2121	G
1	1A	2123	G
1	1A	2126	A
1	1A	2127	G

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Mol	Chain	Res	Type
1	1A	2129	C
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	2140	C
1	1A	2142	C
1	1A	2143	C
1	1A	2144	U
1	1A	2146	C
1	1A	2149	G
1	1A	2150	U
1	1A	2151	G
1	1A	2156	G
1	1A	2157	G
1	1A	2158	A
1	1A	2159	G
1	1A	2165	G
1	1A	2166	G
1	1A	2169	A
1	1A	2172	U
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	2190	G
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	2280	G

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Mol	Chain	Res	Type
1	1A	2283	C
1	1A	2287	A
1	1A	2305	A
1	1A	2308	G
1	1A	2320	A
1	1A	2321	G
1	1A	2325	G
1	1A	2334	G
1	1A	2347	C
1	1A	2350	C
1	1A	2354	G
1	1A	2361	A
1	1A	2383	G
1	1A	2385	C
1	1A	2400	G
1	1A	2406	U
1	1A	2422	A
1	1A	2423	U
1	1A	2425	A
1	1A	2429	G
1	1A	2430	A
1	1A	2431	U
1	1A	2434	A
1	1A	2435	A
1	1A	2439	A
1	1A	2441	C
1	1A	2448	A
1	1A	2468	G
1	1A	2476	A
1	1A	2478	A
1	1A	2491	U
1	1A	2502	G
1	1A	2504	U
1	1A	2505	G
1	1A	2518	A
1	1A	2529	G
1	1A	2535	G
1	1A	2550	G
1	1A	2554	U
1	1A	2566	A
1	1A	2567	G
1	1A	2573	C

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Mol	Chain	Res	Type
1	1A	2574	G
1	1A	2602	A
1	1A	2609	U
1	1A	2611	U
1	1A	2612	C
1	1A	2629	A
1	1A	2630	G
1	1A	2654	A
1	1A	2689	U
1	1A	2690	C
1	1A	2691	C
1	1A	2703	C
1	1A	2712(A)	A
1	1A	2713	A
1	1A	2714	G
1	1A	2726	U
1	1A	2733	A
1	1A	2757	A
1	1A	2758	A
1	1A	2765	A
1	1A	2778	A
1	1A	2790	A
1	1A	2791	C
1	1A	2793	G
1	1A	2794	C
1	1A	2802	G
1	1A	2803	C
1	1A	2820	A
1	1A	2821	A
1	1A	2835	A
1	1A	2872	G
1	1A	2880	C
1	1A	2882	A
1	1A	2892	A
1	1A	2894	G
1	1A	2895	U
2	1B	2	C
2	1B	32	C
2	1B	56	G
2	1B	67	G
2	1B	73	A
2	1B	106	G

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Mol	Chain	Res	Type
2	1B	110	G
32	1a	7	G
32	1a	9	G
32	1a	32	A
32	1a	39	G
32	1a	47	C
32	1a	48	C
32	1a	51	A
32	1a	52	G
32	1a	61	G
32	1a	76	C
32	1a	79	G
32	1a	91	C
32	1a	98	G
32	1a	101	A
32	1a	105	G
32	1a	111	G
32	1a	116	A
32	1a	117	G
32	1a	121	C
32	1a	131	C
32	1a	144	G
32	1a	162	A
32	1a	163	C
32	1a	174	C
32	1a	180	U
32	1a	182	U
32	1a	189(C)	C
32	1a	189(J)	G
32	1a	195	A
32	1a	197	A
32	1a	199	G
32	1a	202	U
32	1a	203	U
32	1a	204	U
32	1a	222	U
32	1a	231	G
32	1a	247	G
32	1a	251	G
32	1a	266	G
32	1a	267	C
32	1a	289	G

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Mol	Chain	Res	Type
32	1a	328	C
32	1a	329	A
32	1a	332	G
32	1a	344	A
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	384	G
32	1a	397	A
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	452	A
32	1a	461	A
32	1a	470	C
32	1a	483	C
32	1a	485	G
32	1a	492	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	521	G
32	1a	524	G
32	1a	527	G7M
32	1a	531	U
32	1a	532	A
32	1a	547	A
32	1a	559	A

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Mol	Chain	Res	Type
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	596	C
32	1a	627	G
32	1a	630	G
32	1a	634	C
32	1a	653	A
32	1a	662	G
32	1a	665	A
32	1a	687	A
32	1a	688	G
32	1a	695	A
32	1a	722	A
32	1a	723	U
32	1a	731	G
32	1a	749	C
32	1a	752	G
32	1a	755	G
32	1a	766	A
32	1a	777	A
32	1a	787	A
32	1a	792	A
32	1a	793	U
32	1a	794	A
32	1a	816	A
32	1a	817	C
32	1a	821	G
32	1a	828	A
32	1a	840	C
32	1a	841	U
32	1a	851	G
32	1a	870	U
32	1a	914	A
32	1a	926	G
32	1a	927	G
32	1a	934	C
32	1a	935	A
32	1a	942	G

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Mol	Chain	Res	Type
32	1a	960	U
32	1a	961	U
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	972	C
32	1a	974	A
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	978	A
32	1a	983	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	1009	G
32	1a	1016	A
32	1a	1020	U
32	1a	1022	G
32	1a	1023	G
32	1a	1026	G
32	1a	1027	C
32	1a	1028	C
32	1a	1030	C
32	1a	1030(A)	G
32	1a	1030(C)	G
32	1a	1031	G
32	1a	1043	C
32	1a	1044	A
32	1a	1068	G
32	1a	1081	G
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1111	A
32	1a	1123	A
32	1a	1124	G
32	1a	1125	U

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Mol	Chain	Res	Type
32	1a	1132	C
32	1a	1133	G
32	1a	1134	G
32	1a	1135	U
32	1a	1137	C
32	1a	1138	G
32	1a	1139	G
32	1a	1140	C
32	1a	1146	A
32	1a	1152	A
32	1a	1159	U
32	1a	1183	A
32	1a	1184	G
32	1a	1196	U
32	1a	1197	G
32	1a	1201	A
32	1a	1202	G
32	1a	1213	A
32	1a	1214	C
32	1a	1227	A
32	1a	1236	A
32	1a	1238	A
32	1a	1250	A
32	1a	1253	G
32	1a	1256	A
32	1a	1257	U
32	1a	1258	G
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	1319	A
32	1a	1338	G
32	1a	1346	A
32	1a	1347	G

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Mol	Chain	Res	Type
32	1a	1350	A
32	1a	1353	G
32	1a	1363	C
32	1a	1364	U
32	1a	1365	G
32	1a	1370	G
32	1a	1377	A
32	1a	1379	G
32	1a	1400	5MC
32	1a	1419	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1446	U
32	1a	1447	A
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
53	1v	13	A
53	1v	14	A
54	1w	2	C
54	1w	5	G
54	1w	8	4SU
54	1w	14	A
54	1w	15	A
54	1w	18	G
54	1w	19	U
54	1w	21	A
54	1w	23	A
54	1w	24	A
54	1w	26	G
54	1w	27	A
54	1w	31	C
54	1w	45	U
54	1w	46	A
54	1w	48	C
54	1w	49	G
54	1w	51	G

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Mol	Chain	Res	Type
54	1w	56	C
54	1w	62	C
54	1w	66	C
54	1w	67	G
54	1w	69	C
54	1w	70	C
54	1w	71	G
54	1w	73	U
54	1w	74	C
55	1x	2	G
55	1x	9	G
55	1x	18	G
55	1x	19	G
55	1x	46	G
55	1x	47	U
55	1x	61	C
56	1y	4	G
56	1y	5	G
56	1y	7	G
56	1y	9	A
56	1y	13	C
56	1y	14	A
56	1y	18	G
56	1y	19	U
56	1y	21	A
56	1y	33	U
56	1y	34	C
56	1y	35	C
56	1y	37	A
56	1y	40	C
56	1y	44	A
56	1y	45	U
56	1y	46	A
56	1y	48	C
56	1y	49	G
56	1y	50	A
56	1y	57	G
56	1y	58	A
56	1y	59	U
56	1y	60	U
56	1y	61	C
56	1y	65	U

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Mol	Chain	Res	Type
56	1y	69	C
56	1y	70	C
56	1y	71	G
1	2A	14	A
1	2A	15	G
1	2A	34	C
1	2A	35	G
1	2A	45	C
1	2A	49	A
1	2A	61	G
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	84	A
1	2A	90	U
1	2A	94	C
1	2A	100	G
1	2A	102	G
1	2A	118	A
1	2A	119	A
1	2A	120	U
1	2A	131	G
1	2A	154	G
1	2A	154(A)	C
1	2A	157	U
1	2A	173	G
1	2A	181	A
1	2A	196	A
1	2A	199	A
1	2A	205	G
1	2A	214	G
1	2A	215	G
1	2A	216	A
1	2A	221	A
1	2A	222	A
1	2A	228	A
1	2A	229	A
1	2A	230	U
1	2A	232	G
1	2A	233	A
1	2A	248	G
1	2A	266	G

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Mol	Chain	Res	Type
1	2A	267	C
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	272	G
1	2A	272(B)	G
1	2A	277	C
1	2A	278	A
1	2A	311	A
1	2A	324	A
1	2A	327	G
1	2A	329	G
1	2A	330	A
1	2A	352	G
1	2A	358	U
1	2A	363(B)	G
1	2A	386	G
1	2A	403	U
1	2A	411	G
1	2A	412	A
1	2A	422	A
1	2A	444	C
1	2A	454	A
1	2A	455	C
1	2A	457	A
1	2A	481	G
1	2A	504	U
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	551	G
1	2A	563	G
1	2A	573	G
1	2A	575	A
1	2A	586	A

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Mol	Chain	Res	Type
1	2A	588	U
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	614(B)	G
1	2A	614(C)	A
1	2A	615	G
1	2A	616	G
1	2A	627	A
1	2A	637	A
1	2A	645	C
1	2A	652(B)	A
1	2A	652(C)	G
1	2A	653	A
1	2A	669	G
1	2A	686	G
1	2A	717	G
1	2A	726	G
1	2A	730	C
1	2A	752	A
1	2A	753	C
1	2A	775	G
1	2A	776	G
1	2A	782	A
1	2A	784	A
1	2A	785	G
1	2A	792	G
1	2A	805	G
1	2A	812	C
1	2A	819	A
1	2A	827	U
1	2A	828	U
1	2A	832	G
1	2A	857	C
1	2A	859	G
1	2A	868	U
1	2A	874	G
1	2A	879	G
1	2A	880	G
1	2A	882	G
1	2A	884	C
1	2A	886	C

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Mol	Chain	Res	Type
1	2A	887	A
1	2A	888	C
1	2A	889	C
1	2A	893	C
1	2A	894	C
1	2A	896	A
1	2A	897	C
1	2A	900	A
1	2A	901	A
1	2A	910	A
1	2A	917	A
1	2A	932	G
1	2A	938	G
1	2A	941	A
1	2A	945	A
1	2A	946	G
1	2A	953	A
1	2A	961	C
1	2A	974	G
1	2A	975	C
1	2A	983	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	1033	U
1	2A	1038	C
1	2A	1039	G
1	2A	1041	C
1	2A	1043	C
1	2A	1114	G
1	2A	1116	C
1	2A	1117	G
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1139	G

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Mol	Chain	Res	Type
1	2A	1142(A)	A
1	2A	1169	G
1	2A	1171	G
1	2A	1210	A
1	2A	1211	U
1	2A	1212	G
1	2A	1220	A
1	2A	1230	C
1	2A	1236	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	1359	A
1	2A	1360	A
1	2A	1365	A
1	2A	1368	G
1	2A	1370	C
1	2A	1373	A
1	2A	1378	A
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	1460	A
1	2A	1466	G
1	2A	1467	C

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Mol	Chain	Res	Type
1	2A	1471	A
1	2A	1482	G
1	2A	1490	A
1	2A	1493	C
1	2A	1494	A
1	2A	1496	A
1	2A	1497	U
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1531	C
1	2A	1532	C
1	2A	1543	C
1	2A	1547	C
1	2A	1558	A
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1580	A
1	2A	1583	A
1	2A	1584	C
1	2A	1608	A
1	2A	1609	A
1	2A	1610	A
1	2A	1648	C
1	2A	1654	A
1	2A	1674	G
1	2A	1696	G
1	2A	1700	A
1	2A	1701	A
1	2A	1703	G
1	2A	1721	G
1	2A	1722	A
1	2A	1740	G
1	2A	1746	G
1	2A	1747	G
1	2A	1756	G
1	2A	1763	G
1	2A	1764	G
1	2A	1769	G
1	2A	1773	A
1	2A	1780	A

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Mol	Chain	Res	Type
1	2A	1782	C
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1812	A
1	2A	1816	G
1	2A	1828	G
1	2A	1829	A
1	2A	1835	G
1	2A	1836	C
1	2A	1847	A
1	2A	1848	A
1	2A	1877	A
1	2A	1878	G
1	2A	1900	A
1	2A	1906	G
1	2A	1913	A
1	2A	1914	C
1	2A	1929	G
1	2A	1930	G
1	2A	1936	A
1	2A	1937	A
1	2A	1938	A
1	2A	1955	U
1	2A	1963	U
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1992	G
1	2A	1993	U
1	2A	1997	G
1	2A	2020	A
1	2A	2023	G
1	2A	2031	A
1	2A	2032	G
1	2A	2033	A
1	2A	2043	C
1	2A	2055	C
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G

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Mol	Chain	Res	Type
1	2A	2063	C
1	2A	2069	G
1	2A	2099	U
1	2A	2110	G
1	2A	2111	C
1	2A	2112	G
1	2A	2116	G
1	2A	2117	A
1	2A	2120	G
1	2A	2122	U
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	2142	C
1	2A	2145	C
1	2A	2146	C
1	2A	2149	G
1	2A	2151	G
1	2A	2156	G
1	2A	2157	G
1	2A	2158	A
1	2A	2159	G
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	2181	G
1	2A	2183	C
1	2A	2186	G

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Mol	Chain	Res	Type
1	2A	2188	C
1	2A	2189	U
1	2A	2192	G
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2218	U
1	2A	2225	A
1	2A	2238	G
1	2A	2239	G
1	2A	2269	A
1	2A	2275	C
1	2A	2278	A
1	2A	2283	C
1	2A	2287	A
1	2A	2288	A
1	2A	2298	A
1	2A	2305	A
1	2A	2308	G
1	2A	2312	U
1	2A	2319	G
1	2A	2320	A
1	2A	2325	G
1	2A	2334	G
1	2A	2336	A
1	2A	2347	C
1	2A	2350	C
1	2A	2354	G
1	2A	2376	A
1	2A	2383	G
1	2A	2385	C
1	2A	2402	C
1	2A	2406	U
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	2465	C

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Mol	Chain	Res	Type
1	2A	2469	A
1	2A	2476	A
1	2A	2491	U
1	2A	2494	G
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	2530	A
1	2A	2554	U
1	2A	2555	U
1	2A	2566	A
1	2A	2567	G
1	2A	2573	C
1	2A	2578	G
1	2A	2602	A
1	2A	2609	U
1	2A	2611	U
1	2A	2612	C
1	2A	2615	U
1	2A	2630	G
1	2A	2654	A
1	2A	2689	U
1	2A	2690	C
1	2A	2691	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	2751	G
1	2A	2764	A
1	2A	2765	A
1	2A	2766	G
1	2A	2778	A
1	2A	2789	C
1	2A	2793	G
1	2A	2794	C

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Mol	Chain	Res	Type
1	2A	2802	G
1	2A	2803	C
1	2A	2804	C
1	2A	2805	G
1	2A	2820	A
1	2A	2821	A
1	2A	2835	A
1	2A	2839	G
1	2A	2872	G
1	2A	2880	C
1	2A	2892	A
1	2A	2894	G
1	2A	2897	U
2	2B	2	C
2	2B	5	C
2	2B	8	U
2	2B	12	C
2	2B	13	A
2	2B	15	A
2	2B	17	C
2	2B	19	G
2	2B	20	C
2	2B	33	G
2	2B	41	U
2	2B	42	C
2	2B	53	A
2	2B	56	G
2	2B	67	G
2	2B	73	A
2	2B	74	U
2	2B	75	G
2	2B	85	G
2	2B	89	G
2	2B	110	G
2	2B	116	G
2	2B	120	A
32	2a	9	G
32	2a	22	G
32	2a	32	A
32	2a	39	G
32	2a	47	C
32	2a	48	C

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Mol	Chain	Res	Type
32	2a	50	A
32	2a	51	A
32	2a	66	G
32	2a	73	G
32	2a	88	A
32	2a	89	C
32	2a	101	A
32	2a	112	G
32	2a	116	A
32	2a	121	C
32	2a	129(A)	G
32	2a	131	C
32	2a	143	A
32	2a	144	G
32	2a	162	A
32	2a	163	C
32	2a	182	U
32	2a	185	A
32	2a	189(F)	U
32	2a	189(J)	G
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	217	C
32	2a	247	G
32	2a	250	A
32	2a	251	G
32	2a	266	G
32	2a	267	C
32	2a	279	A
32	2a	281	G
32	2a	289	G
32	2a	306	G
32	2a	318	G
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	351	G
32	2a	352	C

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Mol	Chain	Res	Type
32	2a	353	A
32	2a	354	G
32	2a	367	U
32	2a	372	C
32	2a	373	A
32	2a	384	G
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	411	A
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	430	A
32	2a	439	A
32	2a	442	C
32	2a	452	A
32	2a	470	C
32	2a	471	G
32	2a	484	G
32	2a	485	G
32	2a	496	A
32	2a	498	U
32	2a	505	G
32	2a	509	A
32	2a	510	A
32	2a	511	C
32	2a	518	C
32	2a	531	U
32	2a	532	A
32	2a	533	A
32	2a	547	A
32	2a	559	A
32	2a	564	C
32	2a	567	G
32	2a	568	G
32	2a	572	A
32	2a	573	A
32	2a	576	G

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Mol	Chain	Res	Type
32	2a	577	G
32	2a	596	C
32	2a	597	G
32	2a	601	C
32	2a	607	A
32	2a	630	G
32	2a	653	A
32	2a	657	G
32	2a	665	A
32	2a	687	A
32	2a	688	G
32	2a	721	G
32	2a	723	U
32	2a	731	G
32	2a	733	A
32	2a	746	A
32	2a	748	C
32	2a	749	C
32	2a	755	G
32	2a	760	G
32	2a	763	G
32	2a	764	C
32	2a	777	A
32	2a	787	A
32	2a	792	A
32	2a	793	U
32	2a	794	A
32	2a	816	A
32	2a	817	C
32	2a	821	G
32	2a	828	A
32	2a	840	C
32	2a	841	U
32	2a	851	G
32	2a	853	G
32	2a	859	A
32	2a	874	G
32	2a	875	C
32	2a	887	G
32	2a	902	G
32	2a	914	A
32	2a	926	G

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Mol	Chain	Res	Type
32	2a	927	G
32	2a	931	C
32	2a	933	G
32	2a	934	C
32	2a	935	A
32	2a	942	G
32	2a	958	A
32	2a	960	U
32	2a	961	U
32	2a	968	A
32	2a	969	A
32	2a	971	G
32	2a	974	A
32	2a	975	A
32	2a	976	G
32	2a	977	A
32	2a	991	U
32	2a	992	U
32	2a	993	G
32	2a	994	A
32	2a	995	C
32	2a	997	U
32	2a	998	G
32	2a	999	C
32	2a	1001	A
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	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

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Mol	Chain	Res	Type
32	2a	1031	G
32	2a	1032	G
32	2a	1033	G
32	2a	1035	A
32	2a	1039	C
32	2a	1040	U
32	2a	1043	C
32	2a	1046	A
32	2a	1050	G
32	2a	1051	C
32	2a	1053	G
32	2a	1064	G
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1071	C
32	2a	1077	G
32	2a	1079	G
32	2a	1081	G
32	2a	1086	U
32	2a	1094	G
32	2a	1095	U
32	2a	1101	A
32	2a	1105	A
32	2a	1113	C
32	2a	1122	U
32	2a	1125	U
32	2a	1126	U
32	2a	1129	C
32	2a	1130	A
32	2a	1133	G
32	2a	1134	G
32	2a	1135	U
32	2a	1136	U
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G
32	2a	1143	G
32	2a	1146	A
32	2a	1147	C
32	2a	1152	A
32	2a	1154	G

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Mol	Chain	Res	Type
32	2a	1157	A
32	2a	1159	U
32	2a	1182	G
32	2a	1184	G
32	2a	1192	C
32	2a	1193	G
32	2a	1196	U
32	2a	1197	G
32	2a	1202	G
32	2a	1211	U
32	2a	1213	A
32	2a	1227	A
32	2a	1228	C
32	2a	1238	A
32	2a	1240	U
32	2a	1241	G
32	2a	1256	A
32	2a	1257	U
32	2a	1260	C
32	2a	1261	A
32	2a	1264	C
32	2a	1267	C
32	2a	1268	A
32	2a	1270	C
32	2a	1273	G
32	2a	1277	C
32	2a	1279	A
32	2a	1280	A
32	2a	1287	A
32	2a	1299	A
32	2a	1302	U
32	2a	1303	C
32	2a	1305	G
32	2a	1306	A
32	2a	1320	C
32	2a	1323	G
32	2a	1338	G
32	2a	1339	A
32	2a	1340	A
32	2a	1346	A
32	2a	1347	G
32	2a	1353	G

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Mol	Chain	Res	Type
32	2a	1358	U
32	2a	1363	C
32	2a	1368	G
32	2a	1370	G
32	2a	1397	C
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1447	A
32	2a	1452	C
32	2a	1456	G
32	2a	1457	G
32	2a	1492	A
32	2a	1494	G
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
53	2v	13	A
53	2v	14	A
54	2w	2	C
54	2w	5	G
54	2w	6	C
54	2w	8	4SU
54	2w	9	A
54	2w	10	G
54	2w	11	U
54	2w	12	U
54	2w	13	C
54	2w	14	A
54	2w	18	G
54	2w	22	G
54	2w	23	A
54	2w	24	A
54	2w	25	C
54	2w	26	G
54	2w	27	A
54	2w	36	C
54	2w	46	A

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Mol	Chain	Res	Type
54	2w	49	G
54	2w	53	G
54	2w	56	C
54	2w	57	G
54	2w	61	C
54	2w	62	C
54	2w	64	U
54	2w	69	C
54	2w	70	C
54	2w	72	C
54	2w	73	U
54	2w	74	C
55	2x	4	G
55	2x	9	G
55	2x	18	G
55	2x	19	G
55	2x	21	A
55	2x	47	U
55	2x	63	G
56	2y	4	G
56	2y	5	G
56	2y	7	G
56	2y	15	A
56	2y	18	G
56	2y	19	U
56	2y	21	A
56	2y	22	G
56	2y	23	A
56	2y	25	C
56	2y	26	G
56	2y	27	A
56	2y	29	A
56	2y	33	U
56	2y	34	C
56	2y	37	A
56	2y	40	C
56	2y	45	U
56	2y	46	A
56	2y	49	G
56	2y	52	G
56	2y	53	G
56	2y	55	PSU

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Mol	Chain	Res	Type
56	2y	56	C
56	2y	57	G
56	2y	58	A
56	2y	59	U
56	2y	61	C
56	2y	62	C
56	2y	66	C
56	2y	67	G
56	2y	69	C
56	2y	70	C
56	2y	73	U
56	2y	75	C

All (57) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	195	A
1	1A	196	A
1	1A	266	G
1	1A	271(K)	U
1	1A	278	A
1	1A	548	A
1	1A	573	G
1	1A	746	A
1	1A	764	A
1	1A	774	A
1	1A	827	U
1	1A	974	G
1	1A	1067	A
1	1A	1142(A)	A
1	1A	1174	A
1	1A	1176	G
1	1A	1442	G
1	1A	1508	A
1	1A	1608	A
1	1A	1762	A
1	1A	1992	G
1	1A	2126	A
1	1A	2134	A
1	1A	2181	G
1	1A	2183	C
1	1A	2406	U

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Mol	Chain	Res	Type
1	1A	2422	A
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(K)	U
1	2A	271(M)	G
1	2A	277	C
1	2A	528	A
1	2A	752	A
1	2A	774	A
1	2A	827	U
1	2A	856	C
1	2A	900	A
1	2A	1210	A
1	2A	1378	A
1	2A	1420	U
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	2156	G
1	2A	2406	U
1	2A	2439	A
1	2A	2689	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	G7M	1a	527	57,32	20,26,27	1.19	2 (10%)	17,39,42	0.66	0
32	M2G	1a	966	32	20,27,28	1.45	3 (15%)	22,40,43	1.01	2 (9%)
1	5MC	2A	1942	1	18,22,23	0.98	2 (11%)	26,32,35	1.13	2 (7%)
55	4SU	1x	8	55	18,21,22	2.13	6 (33%)	26,30,33	1.66	6 (23%)
55	31H	2x	76	55,57	28,34,35	1.01	3 (10%)	23,47,50	1.71	4 (17%)
1	PSU	2A	2605	1	18,21,22	1.30	2 (11%)	22,30,33	1.80	4 (18%)
32	5MC	1a	967	32	18,22,23	0.94	2 (11%)	26,32,35	1.15	2 (7%)
54	L3X	2w	76	54,1	21,28,29	1.42	4 (19%)	15,40,43	1.61	1 (6%)
32	M2G	2a	966	32	20,27,28	1.42	3 (15%)	22,40,43	0.99	2 (9%)
55	5MU	2x	54	55	19,22,23	1.40	5 (26%)	28,32,35	1.93	6 (21%)
1	2MA	2A	2503	1,57	17,25,26	1.09	2 (11%)	17,37,40	0.99	2 (11%)
55	5MU	1x	54	55,57	19,22,23	1.46	4 (21%)	28,32,35	1.93	5 (17%)
55	PSU	1x	55	55	18,21,22	1.34	2 (11%)	22,30,33	1.91	3 (13%)
1	2MA	1A	2503	1,57	17,25,26	1.04	1 (5%)	17,37,40	0.99	2 (11%)
43	0TD	1l	92	43	7,9,10	4.65	1 (14%)	6,11,13	7.27	2 (33%)
54	4SU	1w	8	54	18,21,22	1.75	5 (27%)	26,30,33	2.04	6 (23%)
55	31H	1x	76	55,57	28,34,35	1.05	3 (10%)	23,47,50	1.68	5 (21%)
32	UR3	2a	1498	32	19,22,23	1.01	2 (10%)	26,32,35	1.48	2 (7%)
32	MA6	1a	1518	32	19,26,27	0.82	0	18,38,41	1.51	2 (11%)
54	5MU	2w	54	54	19,22,23	1.38	4 (21%)	28,32,35	1.64	6 (21%)
32	MA6	1a	1519	32	19,26,27	0.82	0	18,38,41	1.49	2 (11%)
1	5MU	2A	1915	1	19,22,23	1.46	5 (26%)	28,32,35	2.04	5 (17%)
1	OMG	2A	2251	1,55	18,26,27	0.94	1 (5%)	19,38,41	1.13	3 (15%)
32	2MG	2a	1207	32	18,26,27	0.94	1 (5%)	16,38,41	1.00	2 (12%)
32	5MC	2a	1400	32	18,22,23	0.95	2 (11%)	26,32,35	1.11	2 (7%)
1	OMG	1A	2251	1,55,57	18,26,27	1.02	1 (5%)	19,38,41	1.06	3 (15%)
32	5MC	2a	1407	32	18,22,23	0.97	2 (11%)	26,32,35	1.25	3 (11%)
32	4OC	2a	1402	32	20,23,24	0.78	0	26,32,35	1.06	3 (11%)
54	5MU	1w	54	54	19,22,23	1.38	4 (21%)	28,32,35	1.77	6 (21%)
55	PSU	2x	55	55	18,21,22	1.34	2 (11%)	22,30,33	1.90	4 (18%)
1	PSU	2A	1917	1	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
32	MA6	2a	1518	32	19,26,27	0.78	0	18,38,41	1.43	2 (11%)
1	PSU	1A	1917	1	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
1	OMC	1A	1920	1	19,22,23	0.84	0	26,31,34	0.95	1 (3%)
1	5MU	2A	1939	1,57	19,22,23	1.38	5 (26%)	28,32,35	2.36	6 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
43	0TD	2l	92	43	7,9,10	4.76	1 (14%)	6,11,13	3.19	3 (50%)
1	OMU	2A	2552	1,57	19,22,23	1.22	2 (10%)	26,31,34	1.79	5 (19%)
32	UR3	1a	1498	32	19,22,23	0.97	1 (5%)	26,32,35	1.47	2 (7%)
54	L3X	1w	76	54,1	21,28,29	1.45	4 (19%)	15,40,43	1.55	1 (6%)
55	5MC	2x	32	55	18,22,23	0.97	2 (11%)	26,32,35	1.19	3 (11%)
56	4SU	1y	8	56	18,21,22	1.78	5 (27%)	26,30,33	1.63	5 (19%)
56	4SU	2y	8	56	18,21,22	1.60	4 (22%)	26,30,33	2.00	4 (15%)
1	5MC	1A	1942	1	18,22,23	0.98	2 (11%)	26,32,35	1.24	2 (7%)
1	OMU	1A	2552	1	19,22,23	1.21	2 (10%)	26,31,34	1.86	6 (23%)
32	2MG	1a	1207	32	18,26,27	0.91	1 (5%)	16,38,41	1.17	3 (18%)
1	5MC	2A	1962	1,57	18,22,23	0.95	2 (11%)	26,32,35	1.12	2 (7%)
1	OMC	2A	1920	1	19,22,23	0.82	0	26,31,34	0.96	1 (3%)
32	G7M	2a	527	57,32	20,26,27	1.26	2 (10%)	17,39,42	0.59	0
32	5MC	1a	1400	32	18,22,23	0.97	2 (11%)	26,32,35	1.18	4 (15%)
56	5MU	2y	54	56	19,22,23	1.49	4 (21%)	28,32,35	1.71	8 (28%)
56	PSU	2y	55	56	18,21,22	1.38	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	2A	1911	1	18,21,22	1.35	2 (11%)	22,30,33	1.84	3 (13%)
32	MA6	2a	1519	32	19,26,27	0.82	0	18,38,41	1.50	2 (11%)
1	PSU	1A	2605	1,57	18,21,22	1.45	3 (16%)	22,30,33	1.85	5 (22%)
55	5MC	1x	32	55	18,22,23	0.97	2 (11%)	26,32,35	1.25	2 (7%)
54	PSU	2w	55	54,57	18,21,22	1.35	2 (11%)	22,30,33	1.92	3 (13%)
1	5MU	1A	1939	1,57	19,22,23	1.47	4 (21%)	28,32,35	2.11	6 (21%)
1	PSU	1A	1911	1	18,21,22	1.41	2 (11%)	22,30,33	1.85	4 (18%)
1	5MC	1A	1962	1	18,22,23	0.99	2 (11%)	26,32,35	1.22	3 (11%)
1	5MU	1A	1915	1	19,22,23	1.39	5 (26%)	28,32,35	2.02	7 (25%)
54	PSU	1w	55	54,57	18,21,22	1.39	2 (11%)	22,30,33	1.85	3 (13%)
32	5MC	1a	1407	32	18,22,23	0.90	2 (11%)	26,32,35	1.15	3 (11%)
32	5MC	1a	1404	32	18,22,23	1.00	2 (11%)	26,32,35	1.25	4 (15%)
56	PSU	1y	55	56	18,21,22	1.35	2 (11%)	22,30,33	1.90	3 (13%)
54	4SU	2w	8	54	18,21,22	1.64	4 (22%)	26,30,33	2.69	5 (19%)
55	4SU	2x	8	55	18,21,22	1.89	5 (27%)	26,30,33	1.31	4 (15%)
32	5MC	2a	1404	32	18,22,23	0.96	2 (11%)	26,32,35	1.13	3 (11%)
32	5MC	2a	967	32	18,22,23	0.96	2 (11%)	26,32,35	1.10	3 (11%)
56	5MU	1y	54	56	19,22,23	1.43	4 (21%)	28,32,35	2.01	6 (21%)
32	PSU	2a	516	32	18,21,22	1.29	2 (11%)	22,30,33	1.79	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	4OC	1a	1402	32	20,23,24	0.74	0	26,32,35	0.89	1 (3%)
32	PSU	1a	516	32	18,21,22	1.40	2 (11%)	22,30,33	1.78	4 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	G7M	1a	527	57,32	-	3/3/25/26	0/3/3/3
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
55	31H	2x	76	55,57	-	5/18/40/41	0/3/3/3
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
54	L3X	2w	76	54,1	-	2/9/31/32	0/3/3/3
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	1,57	-	1/3/25/26	0/3/3/3
55	5MU	1x	54	55,57	-	0/7/25/26	0/2/2/2
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
1	2MA	1A	2503	1,57	-	2/3/25/26	0/3/3/3
43	0TD	1l	92	43	-	1/7/12/14	-
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
55	31H	1x	76	55,57	-	6/18/40/41	0/3/3/3
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/7/29/30	0/3/3/3
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	3/7/29/30	0/3/3/3
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	1,55	-	0/5/27/28	0/3/3/3
32	2MG	2a	1207	32	-	0/5/27/28	0/3/3/3
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
1	OMG	1A	2251	1,55,57	-	0/5/27/28	0/3/3/3
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32	-	2/9/29/30	0/2/2/2
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	0/7/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
1	OMC	1A	1920	1	-	1/9/27/28	0/2/2/2
1	5MU	2A	1939	1,57	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	1/7/12/14	-
1	OMU	2A	2552	1,57	-	0/9/27/28	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
54	L3X	1w	76	54,1	-	0/9/31/32	0/3/3/3
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
56	4SU	1y	8	56	-	0/7/25/26	0/2/2/2
56	4SU	2y	8	56	-	2/7/25/26	0/2/2/2
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
1	OMU	1A	2552	1	-	0/9/27/28	0/2/2/2
32	2MG	1a	1207	32	-	0/5/27/28	0/3/3/3
1	5MC	2A	1962	1,57	-	0/7/25/26	0/2/2/2
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
32	G7M	2a	527	57,32	-	1/3/25/26	0/3/3/3
32	5MC	1a	1400	32	-	2/7/25/26	0/2/2/2
56	5MU	2y	54	56	-	3/7/25/26	0/2/2/2
56	PSU	2y	55	56	-	2/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	3/7/29/30	0/3/3/3
1	PSU	1A	2605	1,57	-	0/7/25/26	0/2/2/2
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
54	PSU	2w	55	54,57	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	1,57	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
1	5MC	1A	1962	1	-	0/7/25/26	0/2/2/2
1	5MU	1A	1915	1	-	0/7/25/26	0/2/2/2
54	PSU	1w	55	54,57	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
56	PSU	1y	55	56	-	2/7/25/26	0/2/2/2
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2
55	4SU	2x	8	55	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	1/7/25/26	0/2/2/2
56	5MU	1y	54	56	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
32	PSU	1a	516	32	-	0/7/25/26	0/2/2/2

All (170) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.27	1.69	1.82
43	1l	92	0TD	CB-SB	-11.77	1.70	1.82
55	1x	8	4SU	C4-N3	-5.02	1.32	1.37
32	1a	966	M2G	C2-N3	4.61	1.36	1.30
32	2a	966	M2G	C2-N3	4.55	1.36	1.30
55	2x	8	4SU	C4-N3	-4.41	1.32	1.37
54	1w	8	4SU	C4-S4	-4.40	1.60	1.68
56	1y	8	4SU	C4-S4	-4.24	1.60	1.68
54	2w	8	4SU	C4-S4	-4.23	1.60	1.68
55	1x	8	4SU	C4-S4	-4.19	1.60	1.68
56	2y	8	4SU	C4-S4	-4.03	1.60	1.68
54	1w	55	PSU	C6-C5	3.98	1.40	1.35
55	1x	8	4SU	C2-N3	-3.93	1.31	1.38
56	2y	55	PSU	C6-C5	3.93	1.39	1.35
54	1w	76	L3X	O4'-C1'	3.85	1.46	1.41
55	2x	8	4SU	C4-S4	-3.83	1.61	1.68
54	2w	55	PSU	C6-C5	3.72	1.39	1.35
56	1y	55	PSU	C6-C5	3.63	1.39	1.35
1	1A	1917	PSU	C6-C5	3.63	1.39	1.35
32	2a	527	G7M	C5-C4	3.63	1.46	1.39
32	1a	527	G7M	C5-C4	3.62	1.46	1.39
1	1A	1911	PSU	C6-C5	3.54	1.39	1.35
32	1a	516	PSU	C6-C5	3.49	1.39	1.35
54	2w	76	L3X	O4'-C1'	3.47	1.45	1.41
55	2x	55	PSU	C6-C5	3.47	1.39	1.35
1	2A	1917	PSU	C6-C5	3.39	1.39	1.35
32	2a	516	PSU	C6-C5	3.35	1.39	1.35
1	1A	2605	PSU	C4-N3	-3.34	1.32	1.38
55	1x	8	4SU	C5-C4	-3.32	1.38	1.42
56	1y	8	4SU	C4-N3	-3.27	1.34	1.37
1	2A	1911	PSU	C6-C5	3.27	1.39	1.35
55	1x	55	PSU	C6-C5	3.13	1.39	1.35
56	2y	54	5MU	C6-C5	3.11	1.39	1.34
56	1y	54	5MU	C6-C5	3.10	1.39	1.34
1	2A	2605	PSU	C6-C5	3.09	1.38	1.35
56	2y	54	5MU	C2-N1	3.04	1.43	1.38
55	2x	8	4SU	C2-N3	-3.04	1.32	1.38
1	1A	1939	5MU	C4-N3	-3.02	1.33	1.38
54	2w	8	4SU	C2-N1	3.01	1.43	1.38
1	2A	1915	5MU	C6-C5	2.98	1.39	1.34
32	1a	1404	5MC	C6-C5	2.94	1.39	1.34
1	2A	1939	5MU	C6-C5	2.92	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	1942	5MC	C6-C5	2.90	1.39	1.34
55	1x	54	5MU	C6-C5	2.90	1.39	1.34
55	2x	54	5MU	C6-C5	2.88	1.39	1.34
54	1w	54	5MU	C6-C5	2.87	1.39	1.34
54	2w	76	L3X	C5-C4	-2.87	1.33	1.40
54	2w	54	5MU	C6-C5	2.85	1.39	1.34
32	2a	1404	5MC	C6-C5	2.85	1.39	1.34
1	1A	1911	PSU	C4-N3	-2.84	1.33	1.38
32	2a	1400	5MC	C6-C5	2.83	1.39	1.34
1	1A	1942	5MC	C6-C5	2.83	1.39	1.34
32	1a	1400	5MC	C6-C5	2.82	1.39	1.34
1	2A	1939	5MU	C4-N3	-2.82	1.33	1.38
54	1w	8	4SU	C5-C4	-2.81	1.38	1.42
1	1A	1939	5MU	C6-N1	-2.79	1.33	1.38
55	2x	76	31H	C5-C4	-2.79	1.33	1.40
32	2a	967	5MC	C6-C5	2.79	1.39	1.34
54	1w	76	L3X	C5-C4	-2.78	1.33	1.40
55	1x	76	31H	C5-C4	-2.78	1.33	1.40
1	1A	1962	5MC	C6-N1	-2.75	1.33	1.38
32	1a	966	M2G	C2-N2	2.74	1.40	1.35
54	1w	8	4SU	C2-N1	2.73	1.42	1.38
32	2a	966	M2G	C2-N2	2.73	1.40	1.35
56	1y	54	5MU	C4-C5	2.72	1.49	1.44
55	2x	32	5MC	C6-C5	2.71	1.39	1.34
32	1a	516	PSU	C4-N3	-2.69	1.33	1.38
55	2x	8	4SU	C5-C4	-2.69	1.39	1.42
1	1A	2605	PSU	C6-C5	2.68	1.38	1.35
1	2A	1962	5MC	C6-C5	2.67	1.39	1.34
1	1A	1939	5MU	C2-N3	-2.67	1.33	1.38
55	1x	54	5MU	C4-N3	-2.65	1.33	1.38
55	1x	32	5MC	C6-C5	2.65	1.39	1.34
55	1x	54	5MU	C2-N1	2.65	1.42	1.38
1	1A	1915	5MU	C4-N3	-2.64	1.33	1.38
1	2A	1915	5MU	C2-N1	2.63	1.42	1.38
54	2w	8	4SU	O2-C2	2.63	1.27	1.23
1	1A	1915	5MU	C6-C5	2.63	1.38	1.34
1	1A	2251	OMG	C6-N1	-2.62	1.34	1.37
1	2A	1915	5MU	C4-C5	2.61	1.49	1.44
54	1w	8	4SU	C4-N3	-2.60	1.34	1.37
55	1x	76	31H	C6-C5	-2.59	1.33	1.43
55	2x	54	5MU	C4-N3	-2.58	1.34	1.38
56	2y	54	5MU	C4-N3	-2.58	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1939	5MU	C6-C5	2.57	1.38	1.34
32	1a	1407	5MC	C6-C5	2.56	1.38	1.34
56	2y	8	4SU	C2-N1	2.55	1.42	1.38
55	2x	76	31H	C6-C5	-2.53	1.33	1.43
1	1A	2552	OMU	C4-N3	-2.53	1.34	1.38
32	2a	1407	5MC	C6-C5	2.51	1.38	1.34
32	1a	966	M2G	C6-N1	-2.50	1.34	1.37
1	2A	1917	PSU	C4-N3	-2.49	1.34	1.38
1	1A	2503	2MA	C2-N3	2.48	1.36	1.31
1	2A	2503	2MA	C2-N3	2.48	1.36	1.31
54	1w	76	L3X	C6-C5	-2.47	1.34	1.43
55	2x	55	PSU	C4-N3	-2.47	1.34	1.38
54	2w	54	5MU	C4-N3	-2.46	1.34	1.38
55	1x	55	PSU	C4-N3	-2.46	1.34	1.38
1	2A	1911	PSU	C4-N3	-2.45	1.34	1.38
54	1w	55	PSU	C4-N3	-2.44	1.34	1.38
56	1y	8	4SU	C5-C4	-2.44	1.39	1.42
32	1a	967	5MC	C6-N1	-2.44	1.33	1.38
32	1a	967	5MC	C6-C5	2.43	1.38	1.34
56	2y	8	4SU	C5-C4	-2.43	1.39	1.42
32	2a	527	G7M	C6-N1	-2.43	1.34	1.37
1	2A	1915	5MU	C4-N3	-2.42	1.34	1.38
1	2A	2605	PSU	C4-N3	-2.42	1.34	1.38
54	1w	54	5MU	C4-C5	2.41	1.48	1.44
54	1w	54	5MU	C4-N3	-2.41	1.34	1.38
1	1A	1962	5MC	C6-C5	2.40	1.38	1.34
54	2w	76	L3X	C6-C5	-2.40	1.34	1.43
32	1a	1207	2MG	C6-N1	-2.39	1.34	1.37
55	1x	32	5MC	C6-N1	-2.39	1.34	1.38
54	2w	55	PSU	C4-N3	-2.39	1.34	1.38
56	1y	8	4SU	C2-N1	2.38	1.42	1.38
54	2w	54	5MU	C2-N1	2.38	1.42	1.38
55	2x	54	5MU	C4-C5	2.37	1.48	1.44
56	1y	55	PSU	C4-N3	-2.37	1.34	1.38
56	1y	8	4SU	C2-N3	-2.35	1.33	1.38
56	2y	8	4SU	C4-N3	-2.35	1.35	1.37
56	1y	54	5MU	C4-N3	-2.34	1.34	1.38
32	2a	1207	2MG	C6-N1	-2.33	1.34	1.37
32	1a	1400	5MC	C6-N1	-2.33	1.34	1.38
32	1a	527	G7M	C6-N1	-2.33	1.34	1.37
1	1A	2605	PSU	C2-N3	-2.32	1.33	1.37
1	2A	1962	5MC	C6-N1	-2.32	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2a	1407	5MC	C6-N1	-2.31	1.34	1.38
54	2w	54	5MU	C4-C5	2.31	1.48	1.44
1	2A	2552	OMU	C4-N3	-2.31	1.34	1.38
1	1A	1942	5MC	C6-N1	-2.30	1.34	1.38
1	1A	1917	PSU	C4-N3	-2.30	1.34	1.38
1	1A	1915	5MU	C2-N1	2.29	1.42	1.38
56	1y	54	5MU	C2-N1	2.28	1.42	1.38
55	1x	54	5MU	C4-C5	2.27	1.48	1.44
32	2a	516	PSU	C4-N3	-2.27	1.34	1.38
1	2A	2552	OMU	C5-C4	2.26	1.48	1.43
54	1w	8	4SU	O2-C2	2.25	1.27	1.23
32	2a	966	M2G	C6-N1	-2.25	1.34	1.37
54	1w	54	5MU	C2-N1	2.23	1.42	1.38
1	1A	1915	5MU	C4-C5	2.23	1.48	1.44
55	2x	32	5MC	C6-N1	-2.20	1.34	1.38
1	2A	1939	5MU	C4-C5	2.20	1.48	1.44
1	2A	1939	5MU	C2-N3	-2.19	1.34	1.38
54	2w	8	4SU	C5-C4	-2.18	1.39	1.42
1	2A	2251	OMG	C6-N1	-2.16	1.34	1.37
54	2w	76	L3X	C5-N7	-2.16	1.31	1.39
56	2y	54	5MU	C4-C5	2.15	1.48	1.44
32	1a	1404	5MC	C6-N1	-2.15	1.34	1.38
55	2x	54	5MU	C2-N3	-2.15	1.34	1.38
1	2A	1942	5MC	C6-N1	-2.14	1.34	1.38
54	1w	76	L3X	C5-N7	-2.14	1.32	1.39
32	2a	1498	UR3	C2-N1	2.13	1.41	1.38
55	1x	76	31H	C5-N7	-2.12	1.32	1.39
55	1x	8	4SU	O2-C2	2.11	1.26	1.23
55	2x	8	4SU	O2-C2	2.11	1.26	1.23
55	2x	76	31H	C5-N7	-2.10	1.32	1.39
56	2y	55	PSU	C4-N3	-2.10	1.34	1.38
1	2A	2503	2MA	C6-N1	-2.10	1.33	1.38
32	2a	1498	UR3	C6-C5	2.09	1.39	1.35
55	2x	54	5MU	C2-N1	2.09	1.41	1.38
32	2a	967	5MC	C6-N1	-2.08	1.34	1.38
1	2A	1915	5MU	C6-N1	-2.08	1.34	1.38
32	1a	1498	UR3	C2-N1	2.07	1.41	1.38
1	2A	1939	5MU	C6-N1	-2.07	1.34	1.38
55	1x	8	4SU	C6-C5	2.06	1.39	1.35
32	2a	1404	5MC	C6-N1	-2.05	1.34	1.38
32	2a	1400	5MC	C6-N1	-2.04	1.34	1.38
1	1A	1915	5MU	C6-N1	-2.03	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2552	OMU	C5-C4	2.02	1.48	1.43
32	1a	1407	5MC	C6-N1	-2.00	1.34	1.38

All (242) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1l	92	0TD	CSB-SB-CB	-17.43	70.91	102.44
54	2w	8	4SU	C4-N3-C2	-8.45	119.13	127.34
43	2l	92	0TD	CSB-SB-CB	-6.73	90.27	102.44
54	2w	8	4SU	C5-C4-N3	6.67	120.88	114.69
1	2A	1917	PSU	N1-C2-N3	6.09	122.03	115.13
55	1x	55	PSU	N1-C2-N3	6.04	121.98	115.13
55	2x	55	PSU	N1-C2-N3	6.04	121.97	115.13
56	1y	55	PSU	N1-C2-N3	6.01	121.94	115.13
32	2a	1498	UR3	C4-N3-C2	-5.99	118.93	124.56
1	2A	1939	5MU	C4-N3-C2	-5.97	119.63	127.35
56	2y	55	PSU	N1-C2-N3	5.96	121.88	115.13
54	2w	55	PSU	N1-C2-N3	5.96	121.88	115.13
54	1w	55	PSU	N1-C2-N3	5.87	121.78	115.13
1	1A	2605	PSU	N1-C2-N3	5.82	121.73	115.13
54	1w	8	4SU	C5-C4-N3	5.80	120.07	114.69
32	1a	1498	UR3	C4-N3-C2	-5.80	119.10	124.56
1	2A	1911	PSU	N1-C2-N3	5.77	121.67	115.13
1	1A	1917	PSU	N1-C2-N3	5.77	121.66	115.13
1	1A	1911	PSU	N1-C2-N3	5.75	121.65	115.13
32	1a	516	PSU	N1-C2-N3	5.68	121.56	115.13
55	2x	76	31H	N3-C2-N1	-5.66	119.83	128.68
56	2y	8	4SU	C4-N3-C2	-5.66	121.84	127.34
55	1x	76	31H	N3-C2-N1	-5.64	119.87	128.68
1	2A	2605	PSU	N1-C2-N3	5.62	121.50	115.13
54	1w	76	L3X	N3-C2-N1	-5.58	119.95	128.68
32	2a	516	PSU	N1-C2-N3	5.58	121.45	115.13
54	2w	76	L3X	N3-C2-N1	-5.55	120.00	128.68
54	2w	8	4SU	C5-C4-S4	-5.42	117.49	124.47
1	2A	1939	5MU	N3-C2-N1	5.37	122.02	114.89
1	1A	2552	OMU	N3-C2-N1	5.35	122.00	114.89
1	2A	1939	5MU	C5-C4-N3	5.32	119.85	115.31
56	2y	8	4SU	C5-C4-N3	5.17	119.48	114.69
54	1w	8	4SU	C4-N3-C2	-5.16	122.33	127.34
56	1y	54	5MU	N3-C2-N1	5.13	121.69	114.89
1	1A	1939	5MU	C4-N3-C2	-5.12	120.72	127.35
1	2A	2552	OMU	N3-C2-N1	5.11	121.67	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1915	5MU	C4-N3-C2	-5.11	120.74	127.35
1	1A	1939	5MU	C5-C4-N3	5.10	119.67	115.31
56	1y	54	5MU	C4-N3-C2	-5.10	120.75	127.35
56	1y	8	4SU	C5-C4-N3	4.99	119.32	114.69
32	1a	1519	MA6	N3-C2-N1	-4.99	120.89	128.68
1	2A	1915	5MU	N3-C2-N1	4.97	121.48	114.89
1	1A	1915	5MU	C4-N3-C2	-4.95	120.94	127.35
1	2A	1939	5MU	C5-C6-N1	-4.94	118.25	123.34
32	2a	1518	MA6	N3-C2-N1	-4.89	121.03	128.68
32	1a	1518	MA6	N3-C2-N1	-4.86	121.08	128.68
55	1x	54	5MU	N3-C2-N1	4.83	121.31	114.89
55	2x	54	5MU	N3-C2-N1	4.77	121.23	114.89
1	1A	1915	5MU	N3-C2-N1	4.77	121.22	114.89
32	2a	1519	MA6	N3-C2-N1	-4.71	121.31	128.68
55	2x	54	5MU	C4-N3-C2	-4.68	121.30	127.35
55	1x	54	5MU	C4-N3-C2	-4.68	121.30	127.35
1	2A	1939	5MU	O4-C4-C5	-4.64	119.53	124.90
1	1A	1939	5MU	C5-C6-N1	-4.63	118.57	123.34
1	1A	1915	5MU	C5-C4-N3	4.62	119.26	115.31
55	1x	8	4SU	C6-C5-C4	-4.51	116.05	119.95
1	2A	2552	OMU	C4-N3-C2	-4.47	120.68	126.58
1	1A	2552	OMU	C4-N3-C2	-4.47	120.69	126.58
54	1w	8	4SU	C5-C4-S4	-4.39	118.82	124.47
1	1A	1939	5MU	N3-C2-N1	4.25	120.53	114.89
56	1y	54	5MU	C5-C4-N3	4.20	118.90	115.31
1	1A	1939	5MU	O4-C4-C5	-4.19	120.04	124.90
1	2A	1915	5MU	C5-C4-N3	4.18	118.88	115.31
55	1x	32	5MC	C5-C6-N1	-4.18	119.03	123.34
55	2x	54	5MU	C5-C4-N3	4.17	118.87	115.31
54	2w	55	PSU	O2-C2-N1	-4.15	118.22	122.79
54	1w	54	5MU	C4-N3-C2	-4.15	121.98	127.35
54	1w	54	5MU	N3-C2-N1	4.11	120.34	114.89
56	2y	55	PSU	O2-C2-N1	-4.04	118.34	122.79
54	1w	54	5MU	C5-C4-N3	4.03	118.75	115.31
55	2x	55	PSU	C4-N3-C2	-4.02	120.54	126.34
32	1a	1404	5MC	C5-C6-N1	-4.02	119.20	123.34
55	1x	54	5MU	C5-C4-N3	4.01	118.74	115.31
1	1A	2605	PSU	C4-N3-C2	-4.01	120.56	126.34
1	1A	1942	5MC	C5-C6-N1	-4.00	119.22	123.34
54	2w	8	4SU	N3-C2-N1	3.97	120.16	114.89
1	2A	2605	PSU	C4-N3-C2	-3.93	120.67	126.34
56	2y	8	4SU	C5-C4-S4	-3.93	119.41	124.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	1y	55	PSU	O2-C2-N1	-3.92	118.47	122.79
54	1w	54	5MU	O4-C4-C5	-3.90	120.38	124.90
56	1y	8	4SU	C4-N3-C2	-3.89	123.56	127.34
1	1A	1911	PSU	C4-N3-C2	-3.88	120.74	126.34
54	2w	8	4SU	O2-C2-N1	-3.88	117.63	122.79
1	2A	1962	5MC	C5-C6-N1	-3.87	119.35	123.34
1	1A	1917	PSU	C4-N3-C2	-3.83	120.81	126.34
1	2A	1911	PSU	C4-N3-C2	-3.83	120.82	126.34
1	2A	1915	5MU	O4-C4-C5	-3.81	120.48	124.90
1	2A	1917	PSU	C4-N3-C2	-3.76	120.92	126.34
55	1x	55	PSU	C4-N3-C2	-3.76	120.92	126.34
55	2x	54	5MU	O4-C4-C5	-3.76	120.55	124.90
54	2w	54	5MU	C5-C4-N3	3.73	118.50	115.31
1	1A	1915	5MU	O4-C4-C5	-3.72	120.59	124.90
1	2A	1915	5MU	C5-C6-N1	-3.70	119.53	123.34
54	2w	54	5MU	N3-C2-N1	3.70	119.80	114.89
56	2y	8	4SU	N3-C2-N1	3.69	119.78	114.89
32	2a	516	PSU	C4-N3-C2	-3.67	121.05	126.34
1	2A	1942	5MC	C5-C6-N1	-3.67	119.56	123.34
54	2w	55	PSU	C4-N3-C2	-3.64	121.09	126.34
32	1a	516	PSU	C4-N3-C2	-3.64	121.09	126.34
56	2y	54	5MU	C5-C4-N3	3.64	118.42	115.31
55	1x	54	5MU	O4-C4-C5	-3.64	120.68	124.90
55	1x	55	PSU	O2-C2-N1	-3.63	118.80	122.79
55	2x	76	31H	O4'-C1'-C2'	-3.62	101.64	106.93
56	2y	54	5MU	N3-C2-N1	3.62	119.69	114.89
56	1y	55	PSU	C4-N3-C2	-3.60	121.16	126.34
54	2w	54	5MU	O4-C4-C5	-3.58	120.75	124.90
1	2A	1917	PSU	O2-C2-N1	-3.57	118.86	122.79
32	1a	1400	5MC	C5-C6-N1	-3.56	119.67	123.34
56	2y	54	5MU	O4-C4-C5	-3.53	120.81	124.90
56	1y	54	5MU	C5-C6-N1	-3.53	119.71	123.34
54	1w	55	PSU	C4-N3-C2	-3.52	121.26	126.34
54	2w	54	5MU	C4-N3-C2	-3.52	122.80	127.35
56	1y	54	5MU	O4-C4-C5	-3.51	120.83	124.90
32	2a	1407	5MC	C5-C6-N1	-3.47	119.77	123.34
56	2y	55	PSU	C4-N3-C2	-3.43	121.40	126.34
54	1w	8	4SU	C1'-N1-C2	3.42	123.77	117.57
32	2a	1400	5MC	C5-C6-N1	-3.41	119.83	123.34
55	1x	54	5MU	C5-C6-N1	-3.41	119.83	123.34
32	1a	1407	5MC	C5-C6-N1	-3.41	119.83	123.34
1	1A	1962	5MC	C5-C6-N1	-3.40	119.84	123.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	1x	8	4SU	O2-C2-N1	3.40	127.31	122.79
55	2x	54	5MU	C5-C6-N1	-3.40	119.84	123.34
1	2A	2552	OMU	O2-C2-N1	-3.38	118.30	122.79
55	2x	32	5MC	C5-C6-N1	-3.36	119.88	123.34
54	1w	55	PSU	O2-C2-N1	-3.31	119.15	122.79
32	2a	967	5MC	C5-C6-N1	-3.30	119.94	123.34
55	1x	8	4SU	S4-C4-N3	-3.30	116.96	120.21
1	1A	2552	OMU	O2-C2-N1	-3.27	118.43	122.79
32	1a	967	5MC	C5-C6-N1	-3.27	119.97	123.34
55	2x	8	4SU	C5-C4-N3	3.27	117.72	114.69
56	2y	54	5MU	C4-N3-C2	-3.27	123.12	127.35
1	1A	1962	5MC	CM5-C5-C6	-3.26	118.49	122.85
1	2A	1939	5MU	O2-C2-N1	-3.26	118.45	122.79
32	2a	1404	5MC	C5-C6-N1	-3.24	120.00	123.34
55	1x	8	4SU	C5-C4-N3	3.20	117.66	114.69
1	2A	1911	PSU	O2-C2-N1	-3.19	119.28	122.79
32	1a	1518	MA6	C4-C5-N7	-3.19	106.08	109.40
32	2a	1519	MA6	C4-C5-N7	-3.14	106.12	109.40
1	1A	1917	PSU	O2-C2-N1	-3.13	119.35	122.79
32	2a	516	PSU	O2-C2-N1	-3.10	119.38	122.79
43	2l	92	0TD	OD2-CG-CB	3.06	119.77	113.15
1	1A	1915	5MU	C5-C6-N1	-3.04	120.21	123.34
56	2y	54	5MU	C1'-N1-C2	3.04	123.07	117.57
1	1A	1911	PSU	O2-C2-N1	-3.00	119.49	122.79
32	2a	1407	5MC	C5-C4-N3	-2.96	118.48	121.67
55	1x	76	31H	O4'-C1'-C2'	-2.95	102.61	106.93
55	2x	55	PSU	O2-C2-N1	-2.95	119.54	122.79
32	1a	1519	MA6	C4-C5-N7	-2.93	106.34	109.40
32	1a	1400	5MC	C5-C4-N3	-2.84	118.61	121.67
55	2x	8	4SU	C6-C5-C4	-2.76	117.56	119.95
43	1l	92	0TD	OD2-CG-CB	2.74	119.07	113.15
32	1a	1207	2MG	C8-N7-C5	2.74	108.20	102.99
1	1A	2552	OMU	O4-C4-C5	-2.70	120.41	125.16
1	2A	2552	OMU	C5-C4-N3	2.69	118.87	114.84
32	2a	1518	MA6	C4-C5-N7	-2.69	106.60	109.40
55	1x	32	5MC	C5-C4-N3	-2.68	118.79	121.67
54	1w	54	5MU	C5-C6-N1	-2.66	120.60	123.34
1	2A	2552	OMU	O4-C4-C5	-2.66	120.49	125.16
1	2A	2503	2MA	C5-C6-N1	2.65	118.59	114.02
56	1y	54	5MU	O2-C2-N1	-2.64	119.28	122.79
32	1a	1407	5MC	O2-C2-N3	-2.63	118.05	122.33
55	2x	8	4SU	C1'-N1-C2	2.60	122.28	117.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2503	2MA	C5-C6-N1	2.58	118.47	114.02
32	1a	1404	5MC	O2-C2-N3	-2.55	118.18	122.33
32	1a	516	PSU	O2-C2-N1	-2.55	119.98	122.79
55	2x	32	5MC	C5-C4-N3	-2.55	118.93	121.67
1	1A	2251	OMG	C5-C6-N1	2.53	118.43	113.95
1	2A	2605	PSU	O2-C2-N1	-2.52	120.01	122.79
1	2A	1942	5MC	C5-C4-N3	-2.52	118.96	121.67
56	2y	54	5MU	C1'-N1-C6	-2.49	116.98	121.12
32	2a	1207	2MG	C8-N7-C5	2.47	107.70	102.99
1	1A	1942	5MC	C5-C4-N3	-2.46	119.02	121.67
32	1a	1404	5MC	C5-C4-N3	-2.45	119.03	121.67
1	2A	1920	OMC	O2-C2-N3	-2.45	118.35	122.33
1	1A	2605	PSU	C5-C6-N1	-2.44	118.44	122.11
55	2x	32	5MC	O2-C2-N3	-2.43	118.38	122.33
56	1y	8	4SU	N3-C2-N1	2.43	118.11	114.89
56	1y	8	4SU	C1'-N1-C2	2.42	121.95	117.57
54	1w	8	4SU	N3-C2-N1	2.42	118.10	114.89
55	2x	76	31H	CA-N-CN	-2.42	119.11	122.82
1	1A	2552	OMU	C5-C4-N3	2.41	118.45	114.84
1	1A	1915	5MU	O2-C2-N1	-2.39	119.61	122.79
32	2a	1404	5MC	C5-C4-N3	-2.38	119.10	121.67
32	1a	1207	2MG	CM2-N2-C2	-2.38	118.60	123.86
1	2A	2503	2MA	C8-N7-C5	2.38	107.53	102.99
1	1A	1915	5MU	C5M-C5-C4	2.38	121.38	118.77
1	1A	2552	OMU	C2'-C1'-N1	-2.37	109.62	114.22
32	1a	966	M2G	C5-C6-N1	2.37	118.14	113.95
1	1A	2503	2MA	C8-N7-C5	2.37	107.51	102.99
1	1A	1962	5MC	C5-C4-N3	-2.36	119.13	121.67
32	1a	1402	4OC	C6-C5-C4	2.36	119.85	116.96
32	2a	966	M2G	C8-N7-C5	2.35	107.46	102.99
56	2y	54	5MU	O2-C2-N3	-2.31	117.19	121.50
56	2y	54	5MU	C5-C6-N1	-2.31	120.96	123.34
32	2a	1407	5MC	O2-C2-N3	-2.31	118.58	122.33
55	1x	76	31H	CA-N-CN	-2.31	119.28	122.82
1	2A	2251	OMG	C5-C6-N1	2.30	118.01	113.95
55	2x	55	PSU	C5-C6-N1	-2.29	118.68	122.11
56	1y	8	4SU	C5-C4-S4	-2.27	121.55	124.47
1	2A	2251	OMG	C8-N7-C5	2.26	107.30	102.99
55	2x	54	5MU	O2-C2-N1	-2.26	119.78	122.79
32	1a	966	M2G	C8-N7-C5	2.26	107.29	102.99
32	2a	967	5MC	C5-C4-N3	-2.26	119.24	121.67
32	1a	1404	5MC	CM5-C5-C6	-2.25	119.84	122.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1407	5MC	C5-C4-N3	-2.25	119.25	121.67
32	2a	1402	4OC	O2-C2-N3	-2.23	118.70	122.33
32	1a	967	5MC	C5-C4-N3	-2.23	119.27	121.67
32	2a	1498	UR3	C3U-N3-C4	2.22	121.07	117.89
32	1a	1207	2MG	C5-C6-N1	2.20	117.84	113.95
32	2a	1402	4OC	CM4-N4-C4	-2.20	118.16	122.45
32	1a	1498	UR3	C6-N1-C2	-2.20	119.82	121.79
55	2x	76	31H	OCN-CN-N	-2.20	119.49	125.27
32	2a	1404	5MC	O2-C2-N3	-2.19	118.77	122.33
55	1x	76	31H	OCN-CN-N	-2.19	119.50	125.27
1	2A	2251	OMG	O6-C6-C5	-2.19	120.10	124.37
54	2w	54	5MU	C5-C6-N1	-2.18	121.10	123.34
54	1w	54	5MU	O2-C2-N1	-2.17	119.89	122.79
1	1A	2251	OMG	O6-C6-C5	-2.17	120.13	124.37
32	2a	1400	5MC	C5-C4-N3	-2.16	119.34	121.67
32	1a	1400	5MC	CM5-C5-C6	-2.16	119.97	122.85
54	2w	54	5MU	C5M-C5-C4	2.15	121.14	118.77
32	1a	1400	5MC	O2-C2-N3	-2.15	118.84	122.33
55	2x	8	4SU	O2-C2-N1	2.15	125.64	122.79
1	1A	2605	PSU	O2-C2-N1	-2.15	120.43	122.79
1	1A	1939	5MU	O2-C2-N1	-2.14	119.94	122.79
32	2a	966	M2G	C5-C6-N1	2.13	117.72	113.95
32	2a	1402	4OC	C6-C5-C4	2.12	119.56	116.96
1	1A	1920	OMC	O2-C2-N3	-2.12	118.88	122.33
1	2A	1962	5MC	C5-C4-N3	-2.12	119.38	121.67
1	1A	2605	PSU	O2-C2-N3	-2.11	117.84	121.82
32	1a	516	PSU	O4'-C1'-C2'	2.09	108.09	105.14
55	1x	76	31H	O2'-C2'-C3'	2.09	116.28	111.16
32	2a	516	PSU	O4'-C1'-C2'	2.09	108.09	105.14
55	1x	8	4SU	O2-C2-N3	-2.08	117.63	121.50
43	2l	92	0TD	OD1-CG-CB	-2.07	118.10	122.44
32	2a	1207	2MG	C5-C6-N1	2.07	117.61	113.95
54	1w	8	4SU	C1'-N1-C6	-2.05	116.36	120.84
1	2A	2605	PSU	C5-C6-N1	-2.05	119.03	122.11
1	1A	1911	PSU	C6-C5-C4	-2.02	116.78	118.20
32	2a	967	5MC	O2-C2-N3	-2.01	119.06	122.33
55	1x	8	4SU	C1'-N1-C2	2.01	121.21	117.57
1	1A	2251	OMG	C8-N7-C5	2.01	106.81	102.99

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	1400	5MC	O4'-C4'-C5'-O5'
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1519	MA6	O4'-C4'-C5'-O5'
54	2w	76	L3X	C3'-C4'-C5'-O5'
54	2w	76	L3X	O4'-C4'-C5'-O5'
55	1x	76	31H	C3'-C4'-C5'-O5'
55	1x	76	31H	N-CA-CB-CG
55	2x	76	31H	C3'-C4'-C5'-O5'
55	2x	76	31H	O4'-C4'-C5'-O5'
56	2y	55	PSU	C3'-C4'-C5'-O5'
56	2y	55	PSU	O4'-C4'-C5'-O5'
32	1a	527	G7M	C3'-C4'-C5'-O5'
32	1a	1400	5MC	C3'-C4'-C5'-O5'
32	1a	1402	4OC	O4'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
32	2a	1402	4OC	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
56	2y	8	4SU	O4'-C4'-C5'-O5'
32	1a	1402	4OC	C3'-C4'-C5'-O5'
32	2a	1402	4OC	C3'-C4'-C5'-O5'
55	1x	76	31H	O4'-C4'-C5'-O5'
55	2x	76	31H	N-CA-CB-CG
56	2y	8	4SU	C3'-C4'-C5'-O5'
55	1x	76	31H	C4'-C5'-O5'-P
32	1a	527	G7M	O4'-C4'-C5'-O5'
55	1x	76	31H	CB-CG-SD-CE
55	1x	76	31H	C-CA-CB-CG
55	2x	76	31H	C-CA-CB-CG
43	2l	92	0TD	CG-CB-SB-CSB
32	2a	527	G7M	C3'-C4'-C5'-O5'
1	2A	2503	2MA	O4'-C4'-C5'-O5'
32	1a	1519	MA6	C4'-C5'-O5'-P
1	1A	2503	2MA	O4'-C4'-C5'-O5'
56	2y	54	5MU	C2'-C1'-N1-C6
32	2a	1519	MA6	C4'-C5'-O5'-P
56	1y	55	PSU	O4'-C1'-C5-C4
56	2y	54	5MU	O4'-C4'-C5'-O5'
43	1l	92	0TD	CG-CB-SB-CSB
56	1y	55	PSU	O4'-C1'-C5-C6
56	2y	54	5MU	C2'-C1'-N1-C2
32	1a	527	G7M	C4'-C5'-O5'-P
32	2a	967	5MC	O4'-C4'-C5'-O5'
1	1A	1920	OMC	C2'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
55	2x	76	31H	C4'-C5'-O5'-P
1	1A	2503	2MA	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2762 ligands modelled in this entry, 2760 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	$\# Z > 2$
60	SF4	1d	501	35	0,12,12	-	-	-		
60	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
60	SF4	1d	501	35	-	-	0/6/5/5
60	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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.51	90 (3%) 49 56	17, 34, 92, 102	0
1	2A	2789/2915 (95%)	0.30	116 (4%) 36 42	32, 55, 90, 102	0
2	1B	120/121 (99%)	0.17	0 100 100	29, 49, 63, 84	0
2	2B	120/121 (99%)	0.09	2 (1%) 70 76	61, 77, 85, 93	0
3	1D	275/276 (99%)	0.64	2 (0%) 87 90	18, 35, 48, 70	0
3	2D	275/276 (99%)	0.81	16 (5%) 23 27	30, 49, 61, 78	0
4	1E	204/206 (99%)	0.51	0 100 100	17, 37, 57, 72	0
4	2E	204/206 (99%)	0.49	6 (2%) 51 59	32, 55, 67, 79	0
5	1F	202/210 (96%)	0.48	1 (0%) 91 94	17, 40, 63, 81	0
5	2F	202/210 (96%)	0.54	3 (1%) 73 79	33, 65, 75, 80	0
6	1G	181/182 (99%)	0.46	5 (2%) 53 60	38, 58, 70, 80	0
6	2G	181/182 (99%)	1.45	57 (31%) 0 0	67, 77, 82, 88	0
7	1H	174/180 (96%)	0.36	1 (0%) 89 92	34, 50, 61, 64	0
7	2H	174/180 (96%)	1.37	46 (26%) 0 0	66, 78, 85, 88	0
8	1I	146/148 (98%)	0.16	0 100 100	45, 70, 78, 83	0
8	2I	146/148 (98%)	0.55	13 (8%) 9 11	54, 71, 79, 81	0
9	1N	140/140 (100%)	0.56	0 100 100	24, 36, 57, 70	0
9	2N	140/140 (100%)	1.01	18 (12%) 3 4	44, 63, 75, 81	0
10	1O	122/122 (100%)	0.56	1 (0%) 86 89	28, 38, 55, 63	0
10	2O	122/122 (100%)	0.60	5 (4%) 37 44	42, 54, 68, 72	0
11	1P	149/150 (99%)	0.50	0 100 100	18, 43, 63, 70	0
11	2P	149/150 (99%)	0.96	21 (14%) 2 3	39, 64, 77, 87	0
12	1Q	141/141 (100%)	0.63	0 100 100	25, 39, 52, 70	0
12	2Q	141/141 (100%)	1.10	27 (19%) 1 1	45, 63, 72, 79	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	0.54	0 100 100	23, 32, 46, 56	0
13	2R	118/118 (100%)	0.50	1 (0%) 86 89	38, 49, 58, 65	0
14	1S	110/112 (98%)	0.38	0 100 100	36, 49, 58, 66	0
14	2S	110/112 (98%)	0.87	16 (14%) 2 3	61, 72, 79, 83	0
15	1T	131/146 (89%)	0.46	1 (0%) 86 89	32, 43, 67, 76	0
15	2T	131/146 (89%)	0.34	0 100 100	46, 57, 72, 77	0
16	1U	116/118 (98%)	0.68	0 100 100	19, 27, 44, 61	0
16	2U	116/118 (98%)	0.68	6 (5%) 27 32	43, 60, 72, 77	0
17	1V	101/101 (100%)	0.47	0 100 100	20, 35, 50, 63	0
17	2V	101/101 (100%)	0.51	6 (5%) 22 26	42, 69, 76, 79	0
18	1W	112/113 (99%)	0.63	0 100 100	22, 30, 49, 71	0
18	2W	112/113 (99%)	0.63	3 (2%) 54 61	38, 47, 65, 78	0
19	1X	95/96 (98%)	0.54	2 (2%) 63 70	25, 37, 57, 75	0
19	2X	95/96 (98%)	0.74	7 (7%) 14 18	45, 57, 73, 82	0
20	1Y	107/110 (97%)	0.38	1 (0%) 84 88	34, 47, 64, 75	0
20	2Y	107/110 (97%)	0.94	12 (11%) 5 7	55, 67, 77, 86	0
21	1Z	154/206 (74%)	0.67	12 (7%) 13 16	39, 61, 83, 86	0
21	2Z	160/206 (77%)	1.38	33 (20%) 1 1	62, 78, 87, 91	0
22	10	83/85 (97%)	0.77	3 (3%) 42 49	27, 36, 51, 64	0
22	20	83/85 (97%)	1.34	18 (21%) 0 0	43, 63, 71, 77	0
23	11	97/98 (98%)	0.60	2 (2%) 63 70	25, 44, 65, 69	0
23	21	97/98 (98%)	0.81	8 (8%) 11 14	39, 54, 71, 76	0
24	12	70/72 (97%)	0.53	0 100 100	33, 46, 57, 72	0
24	22	70/72 (97%)	0.44	0 100 100	58, 67, 76, 79	0
25	13	59/60 (98%)	0.56	0 100 100	26, 33, 55, 70	0
25	23	59/60 (98%)	1.09	10 (16%) 1 1	52, 64, 72, 78	0
26	14	69/71 (97%)	0.57	5 (7%) 15 18	51, 72, 85, 89	0
26	24	69/71 (97%)	1.94	30 (43%) 0 0	74, 83, 89, 93	0
27	15	59/60 (98%)	0.64	1 (1%) 70 76	18, 28, 49, 59	0
27	25	59/60 (98%)	0.54	0 100 100	33, 48, 62, 75	0
28	16	53/54 (98%)	0.49	0 100 100	30, 40, 55, 59	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.69	3 (5%) 23 28	54, 60, 66, 71	0
29	17	48/49 (97%)	0.76	3 (6%) 20 23	19, 26, 51, 58	0
29	27	48/49 (97%)	1.27	8 (16%) 1 1	32, 39, 65, 70	0
30	18	64/65 (98%)	0.57	1 (1%) 72 78	24, 31, 39, 53	0
30	28	64/65 (98%)	1.03	8 (12%) 3 5	44, 56, 63, 65	0
31	19	37/37 (100%)	0.66	0 100 100	29, 37, 53, 55	0
31	29	37/37 (100%)	1.17	6 (16%) 1 2	58, 63, 75, 76	0
32	1a	1488/1521 (97%)	0.08	32 (2%) 62 68	33, 66, 89, 100	0
32	2a	1491/1521 (98%)	0.27	62 (4%) 36 42	48, 75, 92, 102	0
33	1b	231/256 (90%)	0.58	25 (10%) 5 7	59, 74, 82, 88	0
33	2b	231/256 (90%)	1.65	74 (32%) 0 0	73, 82, 87, 92	0
34	1c	206/239 (86%)	0.83	26 (12%) 3 4	58, 70, 78, 85	0
34	2c	206/239 (86%)	1.63	67 (32%) 0 0	70, 82, 86, 89	0
35	1d	208/209 (99%)	1.13	46 (22%) 0 0	53, 68, 76, 82	0
35	2d	208/209 (99%)	0.74	15 (7%) 15 18	60, 70, 77, 81	0
36	1e	148/162 (91%)	0.65	9 (6%) 21 25	46, 62, 71, 76	0
36	2e	148/162 (91%)	1.00	27 (18%) 1 1	67, 74, 81, 83	0
37	1f	100/101 (99%)	0.26	0 100 100	55, 65, 73, 76	0
37	2f	100/101 (99%)	0.31	5 (5%) 28 34	59, 67, 75, 78	0
38	1g	155/156 (99%)	0.60	14 (9%) 9 11	58, 69, 81, 85	0
38	2g	155/156 (99%)	1.42	47 (30%) 0 0	69, 77, 84, 88	0
39	1h	137/138 (99%)	0.51	9 (6%) 18 21	51, 63, 70, 74	0
39	2h	137/138 (99%)	1.14	23 (16%) 1 1	65, 74, 79, 82	0
40	1i	127/128 (99%)	0.83	20 (15%) 2 2	51, 73, 78, 82	0
40	2i	127/128 (99%)	2.33	60 (47%) 0 0	73, 82, 86, 88	0
41	1j	97/105 (92%)	0.70	11 (11%) 5 6	57, 74, 81, 87	0
41	2j	96/105 (91%)	1.71	36 (37%) 0 0	75, 83, 87, 89	0
42	1k	114/129 (88%)	0.80	11 (9%) 8 10	41, 64, 74, 80	0
42	2k	114/129 (88%)	1.34	26 (22%) 0 0	56, 72, 78, 81	0
43	1l	121/132 (91%)	0.70	8 (6%) 18 21	42, 55, 65, 77	0
43	2l	121/132 (91%)	1.29	31 (25%) 0 0	59, 70, 77, 80	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	123/126 (97%)	0.66	10 (8%) 12 15	57, 68, 76, 87	0
44	2m	122/126 (96%)	2.08	46 (37%) 0 0	71, 80, 84, 91	0
45	1n	60/61 (98%)	1.27	7 (11%) 4 6	61, 66, 72, 76	0
45	2n	60/61 (98%)	3.62	46 (76%) 0 0	77, 82, 85, 87	0
46	1o	88/89 (98%)	0.57	5 (5%) 23 28	46, 62, 72, 74	0
46	2o	88/89 (98%)	0.75	6 (6%) 17 20	59, 70, 78, 82	0
47	1p	82/88 (93%)	1.14	14 (17%) 1 1	55, 69, 75, 82	0
47	2p	82/88 (93%)	0.84	8 (9%) 7 9	57, 67, 74, 78	0
48	1q	99/105 (94%)	0.83	7 (7%) 16 19	51, 64, 71, 73	0
48	2q	99/105 (94%)	1.25	23 (23%) 0 0	58, 70, 77, 80	0
49	1r	68/88 (77%)	0.45	3 (4%) 34 41	54, 64, 72, 76	0
49	2r	68/88 (77%)	0.76	8 (11%) 4 6	63, 71, 78, 79	0
50	1s	83/93 (89%)	0.46	3 (3%) 42 49	63, 73, 78, 82	0
50	2s	83/93 (89%)	2.48	45 (54%) 0 0	76, 82, 86, 88	0
51	1t	96/106 (90%)	1.13	23 (23%) 0 0	60, 68, 75, 79	0
51	2t	96/106 (90%)	1.01	16 (16%) 1 1	56, 67, 76, 80	0
52	1u	23/27 (85%)	1.30	7 (30%) 0 0	62, 66, 72, 74	0
52	2u	23/27 (85%)	3.60	17 (73%) 0 0	74, 79, 81, 82	0
53	1v	13/24 (54%)	2.73	7 (53%) 0 0	49, 67, 89, 95	0
53	2v	13/24 (54%)	3.99	10 (76%) 0 0	71, 83, 96, 97	0
54	1w	69/74 (93%)	3.35	50 (72%) 0 0	49, 91, 97, 99	0
54	2w	68/74 (91%)	4.13	59 (86%) 0 0	62, 95, 98, 99	0
55	1x	72/77 (93%)	0.19	1 (1%) 75 81	29, 63, 78, 88	0
55	2x	72/77 (93%)	0.63	9 (12%) 3 5	49, 80, 88, 94	0
56	1y	70/74 (94%)	5.04	68 (97%) 0 0	54, 95, 99, 100	0
56	2y	70/74 (94%)	6.02	70 (100%) 0 0	66, 97, 100, 103	0
All	All	20885/21740 (96%)	0.68	1888 (9%) 9 11	17, 62, 87, 103	0

All (1888) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
44	2m	124	PRO	24.8
44	2m	123	ALA	14.0

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Mol	Chain	Res	Type	RSRZ
44	1m	124	PRO	14.0
56	2y	36	C	13.6
54	2w	71	G	13.4
54	1w	70	C	12.5
56	2y	34	C	11.9
56	1y	34	C	11.8
56	2y	37	A	11.4
45	2n	25	VAL	11.3
45	2n	34	TYR	11.2
56	1y	35	C	10.9
45	2n	39	LEU	10.7
44	2m	122	LYS	10.2
56	1y	36	C	10.2
50	2s	80	TYR	10.0
54	2w	72	C	9.8
33	2b	165	VAL	9.8
56	1y	24	A	9.8
44	1m	123	ALA	9.7
54	1w	3	G	9.6
56	2y	35	C	9.6
56	2y	33	U	9.5
1	2A	2146	C	9.5
53	2v	24	A	9.3
1	2A	2145	C	9.3
1	2A	2111	C	9.2
1	1A	2145	C	9.2
54	1w	71	G	9.1
56	1y	1	G	9.1
56	2y	52	G	8.9
54	2w	1	G	8.8
54	2w	4	G	8.8
56	1y	75	C	8.7
1	2A	2147	G	8.7
56	1y	23	A	8.7
56	2y	17	G	8.7
45	2n	38	GLY	8.7
1	1A	2146	C	8.7
54	1w	4	G	8.6
56	2y	21	A	8.6
1	1A	2159	G	8.5
1	2A	2113	U	8.5
54	2w	2	C	8.4

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Mol	Chain	Res	Type	RSRZ
26	24	49	PHE	8.3
56	2y	57	G	8.3
54	1w	72	C	8.3
56	2y	58	A	8.3
56	1y	39	G	8.2
56	2y	28	G	8.2
21	2Z	149	SER	8.2
38	2g	80	VAL	8.2
6	2G	29	TRP	8.1
38	2g	156	TRP	8.0
56	2y	62	C	8.0
56	1y	2	C	8.0
56	2y	39	G	7.9
1	2A	2802	G	7.9
1	2A	2138	C	7.9
54	2w	70	C	7.9
56	2y	19	U	7.8
56	2y	15	A	7.8
38	1g	80	VAL	7.8
26	24	51	ASP	7.7
56	1y	38	A	7.6
54	2w	56	C	7.6
1	2A	2115	G	7.6
1	2A	2112	G	7.6
56	2y	53	G	7.6
1	2A	2144	U	7.5
44	2m	121	LYS	7.5
56	1y	12	U	7.5
1	2A	2143	C	7.5
32	2a	1030(B)	C	7.5
54	1w	69	C	7.5
52	2u	14	TRP	7.4
1	2A	2154	G	7.4
56	1y	21	A	7.4
40	2i	14	VAL	7.4
1	1A	2140	C	7.4
1	2A	2159	G	7.4
56	2y	74	C	7.3
56	2y	26	G	7.3
56	2y	13	C	7.3
56	1y	22	G	7.3
56	2y	51	G	7.3

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Mol	Chain	Res	Type	RSRZ
1	1A	2147	G	7.3
56	2y	38	A	7.2
1	1A	2112	G	7.1
56	1y	5	G	7.1
1	1A	2113	U	7.1
52	2u	16	GLY	7.1
1	2A	2110	G	7.0
38	1g	79	ARG	7.0
43	2l	64	TYR	7.0
1	2A	2123	G	7.0
56	2y	61	C	7.0
45	2n	29	ARG	7.0
56	2y	14	A	7.0
33	2b	81	VAL	7.0
54	2w	3	G	7.0
1	2A	2167	U	6.9
1	2A	2116	G	6.9
1	1A	2111	C	6.9
1	2A	2170	A	6.9
33	2b	187	LEU	6.9
54	2w	13	C	6.9
54	2w	31	C	6.9
52	2u	13	ILE	6.9
20	2Y	1	MET	6.9
33	2b	37	ASN	6.8
53	2v	13	A	6.8
56	1y	13	C	6.8
21	2Z	139	VAL	6.8
53	1v	24	A	6.8
56	2y	32	U	6.8
44	2m	102	ARG	6.8
56	2y	18	G	6.7
41	2j	65	LEU	6.7
44	2m	7	VAL	6.7
21	2Z	156	LYS	6.6
45	2n	6	LEU	6.6
1	1A	2144	U	6.5
54	2w	10	G	6.5
52	2u	6	ARG	6.5
34	2c	185	GLY	6.5
33	2b	70	PHE	6.5
40	2i	125	TYR	6.5

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Mol	Chain	Res	Type	RSRZ
54	1w	2	C	6.4
56	2y	25	C	6.4
32	2a	1030(A)	G	6.4
1	2A	2117	A	6.4
1	2A	2141	G	6.4
41	2j	47	PHE	6.4
53	1v	13	A	6.4
21	2Z	144	LEU	6.3
56	2y	1	G	6.3
34	2c	8	ILE	6.3
1	1A	2141	G	6.3
45	1n	2	ALA	6.3
38	2g	81	GLY	6.3
56	1y	32	U	6.3
1	2A	2166	G	6.3
54	2w	18	G	6.3
54	2w	39	G	6.3
56	2y	72	C	6.3
38	2g	79	ARG	6.2
50	2s	49	ILE	6.2
34	2c	159	GLY	6.2
54	1w	10	G	6.2
1	2A	2142	C	6.2
56	1y	33	U	6.1
53	2v	23	A	6.1
56	1y	19	U	6.1
9	2N	9	VAL	6.1
1	2A	2801(A)	A	6.1
38	2g	32	ARG	6.1
21	2Z	153	SER	6.1
56	1y	71	G	6.1
26	24	45	GLY	6.1
33	2b	92	TYR	6.1
56	2y	66	C	6.1
54	2w	40	C	6.0
1	1A	2115	G	6.0
33	2b	122	PHE	6.0
1	1A	2130	U	6.0
55	2x	1	C	6.0
38	2g	154	TYR	6.0
40	2i	5	TYR	6.0
1	1A	2160	G	6.0

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Mol	Chain	Res	Type	RSRZ
1	2A	2148	G	6.0
22	20	6	GLY	6.0
34	2c	157	ILE	6.0
1	2A	2160	G	6.0
21	2Z	155	LEU	6.0
56	1y	18	G	5.9
56	2y	30	G	5.9
56	1y	27	A	5.9
56	2y	23	A	5.9
40	2i	127	LYS	5.9
44	2m	90	LEU	5.9
40	2i	123	PRO	5.9
56	2y	64	U	5.9
45	2n	18	VAL	5.9
56	1y	74	C	5.9
1	2A	2155	G	5.9
33	2b	211	ILE	5.9
56	1y	3	G	5.9
33	2b	214	ILE	5.8
1	2A	2114	A	5.8
34	2c	87	LEU	5.8
22	20	2	ALA	5.8
1	2A	2181	G	5.8
32	1a	1030(A)	G	5.8
32	2a	1033	G	5.8
56	2y	63	C	5.8
1	2A	2127	G	5.7
56	2y	56	C	5.7
45	2n	31	ARG	5.7
50	2s	84	GLY	5.7
32	1a	1030(B)	C	5.6
56	2y	2	C	5.6
56	2y	29	A	5.6
56	1y	25	C	5.6
21	1Z	1	MET	5.6
29	27	48	LYS	5.6
45	2n	35	ARG	5.6
32	2a	1034	G	5.6
54	1w	66	C	5.6
38	2g	4	ARG	5.6
1	2A	2168	G	5.6
43	2l	32	PHE	5.6

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Mol	Chain	Res	Type	RSRZ
56	2y	24	A	5.5
38	2g	82	GLY	5.5
54	2w	38	A	5.5
33	2b	216	SER	5.5
6	2G	3	LEU	5.5
39	2h	93	VAL	5.5
56	1y	14	A	5.5
1	1A	2143	C	5.5
1	1A	2117	A	5.4
1	2A	2182	G	5.4
40	2i	114	TYR	5.4
38	1g	153	HIS	5.4
22	20	7	LEU	5.4
1	2A	2179	C	5.4
54	1w	67	G	5.4
56	2y	4	G	5.4
56	2y	22	G	5.4
53	1v	12	A	5.4
56	2y	60	U	5.4
34	2c	180	ALA	5.4
56	1y	56	C	5.3
45	2n	36	PHE	5.3
40	1i	8	GLY	5.3
40	2i	106	ALA	5.3
21	2Z	148	ASP	5.3
33	2b	71	VAL	5.3
34	2c	124	ILE	5.3
1	2A	2135	A	5.3
53	2v	14	A	5.3
23	21	2	SER	5.2
56	2y	5	G	5.2
1	2A	2188	C	5.2
1	2A	2109	U	5.2
26	24	56	VAL	5.2
56	2y	65	U	5.2
1	1A	2109	U	5.2
32	2a	1036	G	5.2
40	2i	10	ARG	5.2
45	2n	22	THR	5.2
22	20	5	LYS	5.1
53	2v	12	A	5.1
22	20	3	HIS	5.1

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Mol	Chain	Res	Type	RSRZ
32	2a	1532	U	5.1
45	2n	2	ALA	5.1
56	1y	72	C	5.1
50	2s	12	ASP	5.1
44	2m	120	LYS	5.1
33	2b	118	LEU	5.1
56	2y	70	C	5.1
1	2A	2169	A	5.1
32	1a	1028	C	5.1
56	1y	31	C	5.1
54	1w	49	G	5.0
40	2i	109	VAL	5.0
56	1y	29	A	5.0
1	2A	2120	G	5.0
39	2h	131	GLY	5.0
54	2w	73	U	5.0
56	2y	12	U	5.0
50	1s	71	LEU	5.0
1	2A	2803	C	5.0
45	2n	42	ILE	5.0
34	2c	194	GLY	5.0
34	2c	184	TYR	5.0
52	2u	15	ARG	5.0
32	1a	1030(C)	G	4.9
1	1A	2132	U	4.9
54	2w	61	C	4.9
33	2b	201	ILE	4.9
33	2b	34	ALA	4.9
45	2n	11	LYS	4.9
32	2a	1257	U	4.9
1	2A	2174	C	4.9
56	1y	70	C	4.9
1	2A	885	C	4.9
1	2A	888	C	4.9
54	1w	13	C	4.9
42	2k	25	TYR	4.9
38	2g	2	ALA	4.9
1	1A	2138	C	4.8
45	2n	37	PHE	4.8
32	2a	1030	C	4.8
54	1w	1	G	4.8
38	1g	81	GLY	4.8

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Mol	Chain	Res	Type	RSRZ
40	2i	36	TYR	4.8
6	2G	139	LEU	4.8
32	1a	204	U	4.8
1	1A	2161	C	4.8
41	2j	67	THR	4.8
50	2s	52	TYR	4.8
33	2b	131	PRO	4.8
44	2m	92	HIS	4.8
1	1A	2129	C	4.8
1	2A	2129	C	4.8
1	1A	2181	G	4.8
56	2y	10	G	4.8
40	2i	115	GLY	4.8
52	2u	11	GLY	4.8
50	2s	50	ALA	4.8
54	2w	50	A	4.7
1	2A	2104	G	4.7
54	1w	5	G	4.7
40	2i	76	ALA	4.7
46	2o	57	LEU	4.7
26	24	63	TYR	4.7
34	2c	13	GLY	4.7
40	2i	126	SER	4.7
56	2y	46	A	4.7
33	2b	152	PHE	4.7
56	2y	71	G	4.7
34	2c	196	LEU	4.7
40	2i	81	ILE	4.7
54	2w	67	G	4.7
56	2y	67	G	4.7
1	1A	2174	C	4.7
36	2e	90	VAL	4.7
50	2s	82	GLY	4.7
56	1y	46	A	4.7
34	2c	182	ILE	4.7
41	2j	38	ILE	4.7
44	2m	4	ILE	4.7
1	2A	2133	G	4.7
21	2Z	96	VAL	4.7
1	1A	1064	C	4.6
50	2s	68	GLY	4.6
54	1w	31	C	4.6

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Mol	Chain	Res	Type	RSRZ
56	1y	49	G	4.6
22	10	7	LEU	4.6
45	2n	23	ARG	4.6
34	2c	60	ALA	4.6
32	1a	1036	G	4.6
1	1A	2114	A	4.6
43	2l	18	VAL	4.6
54	1w	56	C	4.6
41	2j	48	THR	4.6
7	2H	24	VAL	4.6
45	2n	10	ALA	4.6
56	1y	50	A	4.6
21	2Z	143	GLY	4.6
40	2i	59	PHE	4.6
56	1y	63	C	4.6
50	2s	48	THR	4.6
12	2Q	104	PHE	4.6
1	2A	2128	C	4.5
56	2y	42	C	4.5
40	2i	9	ARG	4.5
34	2c	158	GLY	4.5
1	2A	2121	G	4.5
32	1a	1031	G	4.5
48	1q	27	PHE	4.5
50	2s	30	LEU	4.5
56	2y	73	U	4.5
45	2n	61	TRP	4.5
36	2e	12	LEU	4.5
54	2w	5	G	4.5
21	2Z	152	ALA	4.5
1	1A	888	C	4.5
48	1q	98	LEU	4.5
47	2p	19	ILE	4.5
34	2c	160	ALA	4.5
56	2y	31	C	4.5
7	2H	103	LEU	4.5
54	2w	21	A	4.5
1	2A	2793	G	4.5
50	2s	62	ILE	4.5
51	1t	55	ILE	4.5
50	2s	38	SER	4.5
54	1w	14	A	4.5

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Mol	Chain	Res	Type	RSRZ
32	2a	1030(C)	G	4.5
56	1y	30	G	4.5
1	1A	2142	C	4.5
33	2b	127	ILE	4.4
41	2j	62	HIS	4.4
32	1a	1257	U	4.4
44	2m	87	TYR	4.4
38	2g	40	ALA	4.4
6	2G	140	ILE	4.4
56	1y	4	G	4.4
56	1y	28	G	4.4
50	2s	67	VAL	4.4
1	2A	2804	C	4.4
54	2w	30	G	4.4
56	2y	41	U	4.4
52	2u	22	ARG	4.4
41	2j	6	ILE	4.4
56	2y	43	U	4.4
50	2s	63	THR	4.4
35	1d	138	TYR	4.4
7	2H	115	VAL	4.4
3	2D	38	LYS	4.4
56	1y	62	C	4.3
40	2i	7	THR	4.3
32	2a	1220	G	4.3
44	2m	78	ILE	4.3
22	20	4	LYS	4.3
32	2a	1027	C	4.3
38	2g	78	ARG	4.3
33	2b	232	PRO	4.3
56	2y	45	U	4.3
1	2A	2136	C	4.3
44	2m	6	GLY	4.3
44	2m	103	THR	4.3
32	2a	1202	G	4.3
38	2g	6	ARG	4.3
56	1y	42	C	4.3
26	24	57	GLU	4.3
34	2c	6	HIS	4.3
33	2b	228	GLY	4.3
29	27	46	VAL	4.3
26	24	52	THR	4.3

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Mol	Chain	Res	Type	RSRZ
3	2D	2	ALA	4.3
56	1y	66	C	4.2
56	2y	48	C	4.2
1	2A	2122	U	4.2
6	2G	41	GLN	4.2
40	2i	90	PRO	4.2
47	1p	7	ALA	4.2
42	2k	29	ILE	4.2
31	29	37	GLY	4.2
54	2w	23	A	4.2
56	2y	75	C	4.2
34	2c	207	VAL	4.2
44	2m	84	ILE	4.2
14	2S	20	ARG	4.2
1	1A	2133	G	4.2
7	2H	133	VAL	4.2
56	2y	3	G	4.2
47	1p	17	TYR	4.2
6	2G	39	ILE	4.2
40	2i	19	LEU	4.2
40	2i	40	LEU	4.2
56	2y	6	C	4.2
45	2n	13	THR	4.2
35	2d	164	ALA	4.2
56	1y	52	G	4.2
9	2N	112	LEU	4.2
40	2i	17	VAL	4.2
34	2c	193	TYR	4.2
1	1A	2166	G	4.1
40	2i	124	GLN	4.1
1	2A	2180	U	4.1
45	2n	44	LEU	4.1
38	2g	83	ALA	4.1
43	2l	28	LYS	4.1
43	2l	39	VAL	4.1
40	1i	113	LYS	4.1
1	2A	2118	U	4.1
1	2A	2100	G	4.1
54	2w	49	G	4.1
38	2g	9	VAL	4.1
1	2A	2140	C	4.1
34	1c	184	TYR	4.1

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Mol	Chain	Res	Type	RSRZ
54	2w	25	C	4.1
19	2X	92	LEU	4.1
1	2A	2165	G	4.1
32	1a	1001(A)	G	4.1
54	1w	30	G	4.1
1	1A	889	C	4.1
54	1w	25	C	4.1
54	2w	69	C	4.1
1	2A	229	A	4.1
52	2u	5	ASP	4.1
29	27	45	ALA	4.1
44	2m	119	GLY	4.1
56	1y	67	G	4.1
44	2m	60	VAL	4.1
41	2j	63	PHE	4.1
32	2a	1224	G	4.0
44	2m	66	LEU	4.0
33	2b	33	TYR	4.0
54	1w	23	A	4.0
50	2s	41	VAL	4.0
50	2s	31	ILE	4.0
34	2c	80	GLY	4.0
32	2a	1035	A	4.0
38	2g	27	ILE	4.0
12	2Q	32	TYR	4.0
14	2S	35	ILE	4.0
35	1d	157	LEU	4.0
50	2s	15	LEU	4.0
45	1n	51	GLY	4.0
50	2s	79	THR	4.0
42	2k	89	ALA	4.0
21	2Z	141	VAL	4.0
1	1A	2188	C	4.0
32	1a	1029	C	4.0
1	2A	1026	U	4.0
54	2w	11	U	4.0
54	2w	32	U	4.0
7	2H	35	VAL	4.0
32	2a	1114	C	4.0
56	2y	68	C	4.0
7	2H	82	GLY	4.0
56	1y	45	U	4.0

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Mol	Chain	Res	Type	RSRZ
33	2b	130	ARG	4.0
41	2j	60	ARG	4.0
26	24	50	VAL	4.0
33	2b	164	VAL	4.0
41	2j	68	HIS	4.0
45	2n	12	ARG	3.9
1	2A	883	G	3.9
54	1w	32	U	3.9
6	2G	92	VAL	3.9
40	2i	26	VAL	3.9
36	2e	123	LEU	3.9
40	2i	121	ARG	3.9
54	2w	14	A	3.9
54	2w	28	G	3.9
7	2H	105	LEU	3.9
34	2c	33	LEU	3.9
26	24	39	CYS	3.9
56	1y	48	C	3.9
56	1y	73	U	3.9
11	2P	79	ARG	3.9
11	2P	109	GLY	3.9
1	2A	2162	G	3.9
20	2Y	90	LEU	3.9
33	2b	163	PHE	3.9
48	1q	36	ILE	3.9
1	2A	2189	U	3.9
1	2A	2139	C	3.9
12	2Q	121	ALA	3.9
29	27	1	MET	3.9
6	2G	142	PRO	3.9
50	2s	35	SER	3.9
7	2H	107	VAL	3.9
44	2m	15	VAL	3.9
54	2w	24	A	3.9
56	2y	50	A	3.9
52	2u	12	LYS	3.9
1	2A	2149	G	3.9
33	2b	121	LEU	3.9
40	2i	66	ARG	3.9
3	2D	276	LYS	3.9
45	2n	58	LYS	3.9
1	2A	2134	A	3.9

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Mol	Chain	Res	Type	RSRZ
39	2h	112	LEU	3.9
54	2w	15	A	3.9
1	2A	2101	G	3.9
53	2v	21	G	3.9
35	2d	112	VAL	3.9
36	2e	20	GLN	3.9
35	1d	70	ILE	3.8
14	2S	32	LEU	3.8
19	2X	69	TYR	3.8
26	24	32	TYR	3.8
45	2n	53	LEU	3.8
43	2l	56	ALA	3.8
1	1A	2131	G	3.8
44	1m	122	LYS	3.8
1	2A	2164	C	3.8
7	2H	48	GLY	3.8
38	2g	120	ILE	3.8
1	1A	2169	A	3.8
53	2v	15	A	3.8
6	2G	28	VAL	3.8
41	2j	72	VAL	3.8
45	2n	57	ARG	3.8
43	1l	64	TYR	3.8
55	2x	47	U	3.8
56	2y	11	U	3.8
1	2A	2119	A	3.8
33	2b	14	GLY	3.8
44	1m	2	ALA	3.8
54	2w	17	G	3.8
56	2y	69	C	3.8
40	2i	110	GLU	3.8
56	2y	59	U	3.8
14	2S	58	LEU	3.8
44	2m	70	LEU	3.8
33	2b	135	GLN	3.8
40	1i	126	SER	3.8
43	2l	68	ALA	3.8
1	1A	2162	G	3.8
1	2A	2156	G	3.8
25	23	29	ARG	3.8
39	2h	133	LEU	3.8
33	2b	139	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
35	1d	3	ARG	3.7
56	1y	6	C	3.7
21	1Z	102	LEU	3.7
34	1c	87	LEU	3.7
56	1y	68	C	3.7
35	1d	135	LEU	3.7
39	2h	2	LEU	3.7
41	2j	49	VAL	3.7
1	1A	1096	A	3.7
34	2c	65	ALA	3.7
54	1w	24	A	3.7
1	1A	2137	C	3.7
1	2A	884	C	3.7
32	1a	999	C	3.7
54	2w	42	C	3.7
40	2i	49	PRO	3.7
48	2q	9	VAL	3.7
9	2N	8	GLN	3.7
56	1y	53	G	3.7
56	2y	27	A	3.7
8	2I	35	LEU	3.7
14	2S	31	SER	3.7
32	1a	1030	C	3.7
50	2s	71	LEU	3.7
26	14	45	GLY	3.7
34	2c	155	GLY	3.7
6	2G	102	PHE	3.7
29	27	47	ARG	3.7
40	2i	37	PHE	3.7
32	1a	1035	A	3.7
33	2b	210	SER	3.7
40	2i	102	LEU	3.7
34	2c	198	VAL	3.7
32	1a	1034	G	3.7
12	2Q	10	ARG	3.7
41	2j	66	ARG	3.7
43	2l	60	LEU	3.6
54	2w	27	A	3.6
56	1y	51	G	3.6
56	1y	57	G	3.6
52	2u	17	THR	3.6
21	2Z	173	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
56	1y	59	U	3.6
34	1c	201	TYR	3.6
34	2c	178	LEU	3.6
53	1v	23	A	3.6
32	1a	1003	G	3.6
6	2G	136	ARG	3.6
43	2l	13	LYS	3.6
56	1y	60	U	3.6
7	2H	113	VAL	3.6
22	10	6	GLY	3.6
53	2v	22	U	3.6
12	2Q	79	LEU	3.6
56	1y	10	G	3.6
1	1A	1095	A	3.6
38	2g	26	PHE	3.6
43	2l	59	ARG	3.6
32	2a	1031	G	3.6
32	2a	1032	G	3.6
40	1i	14	VAL	3.6
44	2m	101	GLN	3.6
14	2S	3	ARG	3.5
19	2X	68	ARG	3.5
1	2A	2102	U	3.5
56	1y	64	U	3.5
40	2i	105	ASP	3.5
7	2H	102	ALA	3.5
38	1g	156	TRP	3.5
54	2w	29	A	3.5
41	2j	55	LYS	3.5
44	2m	65	LYS	3.5
53	1v	15	A	3.5
1	2A	2175	C	3.5
54	1w	61	C	3.5
26	14	59	PHE	3.5
1	1A	1066	U	3.5
54	2w	26	G	3.5
42	2k	31	THR	3.5
1	1A	2170	A	3.5
3	2D	5	LYS	3.5
1	1A	2139	C	3.5
1	1A	2803	C	3.5
34	2c	206	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
33	2b	227	GLY	3.5
54	2w	57	G	3.5
41	2j	59	SER	3.5
33	1b	215	LEU	3.5
35	1d	21	LEU	3.5
11	2P	32	THR	3.5
40	2i	27	THR	3.5
23	1l	2	SER	3.5
50	2s	13	ASP	3.5
7	2H	52	VAL	3.5
43	1l	18	VAL	3.5
50	2s	53	ASN	3.5
52	2u	21	TYR	3.4
44	2m	42	ALA	3.4
16	2U	17	ILE	3.4
42	1k	25	TYR	3.4
26	24	40	HIS	3.4
40	2i	65	VAL	3.4
1	1A	2118	U	3.4
1	1A	2128	C	3.4
1	2A	2161	C	3.4
38	2g	85	TYR	3.4
40	1i	19	LEU	3.4
41	2j	71	LEU	3.4
7	2H	106	THR	3.4
32	2a	1287	A	3.4
35	1d	180	GLY	3.4
6	2G	5	VAL	3.4
14	2S	29	PHE	3.4
34	1c	39	ILE	3.4
34	1c	81	GLY	3.4
38	1g	84	ASN	3.4
53	1v	14	A	3.4
1	1A	2804	C	3.4
1	2A	2183	C	3.4
54	2w	22	G	3.4
26	24	59	PHE	3.4
34	2c	134	ILE	3.4
48	2q	65	ILE	3.4
51	1t	69	GLY	3.4
7	2H	94	TYR	3.4
20	2Y	55	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
52	2u	8	THR	3.4
11	2P	15	ARG	3.4
6	2G	152	LEU	3.3
7	1H	2	SER	3.3
33	2b	55	PHE	3.3
36	2e	109	ILE	3.3
44	2m	64	TRP	3.3
26	24	43	TYR	3.3
1	2A	2158	A	3.3
9	2N	140	VAL	3.3
56	1y	37	A	3.3
54	1w	39	G	3.3
56	2y	7	G	3.3
12	2Q	66	ILE	3.3
1	2A	2897	U	3.3
40	2i	62	TYR	3.3
21	2Z	145	GLU	3.3
33	1b	229	VAL	3.3
6	2G	34	LEU	3.3
38	2g	22	LEU	3.3
41	2j	40	LEU	3.3
1	2A	882	G	3.3
54	1w	26	G	3.3
36	1e	10	MET	3.3
34	2c	197	GLY	3.3
36	2e	22	GLY	3.3
1	1A	2158	A	3.3
32	2a	1223	C	3.3
36	2e	13	ILE	3.3
49	2r	85	LEU	3.3
52	2u	10	ARG	3.3
33	1b	123	ALA	3.3
20	2Y	5	MET	3.3
45	2n	55	GLY	3.3
1	2A	2105	C	3.3
32	2a	1219	U	3.3
44	1m	98	VAL	3.3
7	2H	123	PHE	3.3
35	1d	111	ALA	3.3
42	2k	117	ASN	3.3
39	2h	58	TYR	3.3
52	2u	23	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
8	2l	75	LEU	3.2
48	2q	60	ILE	3.2
50	2s	47	HIS	3.2
45	2n	26	ARG	3.2
46	2o	60	VAL	3.2
41	1j	47	PHE	3.2
32	2a	1531	A	3.2
11	2P	125	VAL	3.2
9	2N	104	LYS	3.2
45	2n	50	LYS	3.2
33	1b	214	ILE	3.2
54	1w	7	G	3.2
33	2b	233	SER	3.2
1	1A	1509	C	3.2
7	2H	51	ARG	3.2
39	2h	95	VAL	3.2
51	1t	47	GLY	3.2
40	2i	93	ARG	3.2
40	2i	128	ARG	3.2
1	2A	2805	G	3.2
53	2v	20	G	3.2
3	2D	177	LEU	3.2
21	2Z	170	THR	3.2
39	2h	36	LEU	3.2
42	2k	13	GLN	3.2
40	1i	106	ALA	3.2
45	2n	40	CYS	3.2
40	2i	63	ILE	3.2
16	2U	2	PRO	3.2
32	2a	1001(A)	G	3.2
32	2a	1061	G	3.2
56	1y	26	G	3.2
45	2n	17	LYS	3.2
6	2G	80	PHE	3.2
32	1a	1000	U	3.2
40	2i	33	PHE	3.2
41	2j	54	PHE	3.2
50	2s	40	ILE	3.2
33	2b	97	TRP	3.2
6	2G	11	TYR	3.1
32	1a	1026	G	3.1
54	1w	62	C	3.1

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Mol	Chain	Res	Type	RSRZ
26	24	15	ILE	3.1
33	2b	133	LYS	3.1
33	2b	93	VAL	3.1
6	2G	50	ALA	3.1
1	1A	2794	C	3.1
20	2Y	75	ILE	3.1
54	1w	19	U	3.1
1	2A	2319	G	3.1
32	2a	1026	G	3.1
56	2y	49	G	3.1
54	2w	58	A	3.1
56	2y	76	A	3.1
45	2n	41	ARG	3.1
33	2b	123	ALA	3.1
40	2i	108	VAL	3.1
48	2q	95	TYR	3.1
22	20	11	ARG	3.1
34	2c	202	ILE	3.1
1	1A	2120	G	3.1
1	1A	2165	G	3.1
30	28	21	LYS	3.1
17	2V	72	VAL	3.1
21	2Z	174	VAL	3.1
41	2j	44	VAL	3.1
47	1p	21	VAL	3.1
26	24	54	GLY	3.1
35	1d	115	ARG	3.1
44	2m	9	ILE	3.1
50	2s	66	MET	3.1
54	2w	41	U	3.1
56	1y	7	G	3.1
25	23	26	LEU	3.1
25	23	28	LEU	3.1
34	2c	47	LEU	3.1
35	2d	168	ARG	3.1
33	2b	136	VAL	3.1
22	10	3	HIS	3.1
44	2m	82	MET	3.1
54	2w	74	C	3.1
38	2g	155	ARG	3.1
32	2a	1357	A	3.1
35	1d	11	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
46	1o	89	GLY	3.1
56	1y	9	A	3.1
35	1d	203	VAL	3.1
1	1A	2110	G	3.1
50	2s	14	HIS	3.1
45	2n	16	PHE	3.1
51	2t	41	ILE	3.1
23	2l	28	GLY	3.1
38	1g	82	GLY	3.1
43	2l	47	LYS	3.1
11	2P	45	LEU	3.1
12	2Q	2	LEU	3.1
52	1u	17	THR	3.1
35	1d	105	VAL	3.1
33	1b	232	PRO	3.0
26	24	58	ARG	3.0
26	24	68	ARG	3.0
34	2c	186	PHE	3.0
50	2s	81	ARG	3.0
41	1j	57	LYS	3.0
14	2S	5	THR	3.0
40	1i	47	LEU	3.0
54	2w	36	C	3.0
56	2y	40	C	3.0
29	17	46	VAL	3.0
40	2i	73	GLN	3.0
41	1j	44	VAL	3.0
44	2m	104	ARG	3.0
32	1a	171	A	3.0
45	1n	15	LYS	3.0
50	2s	70	LYS	3.0
34	1c	8	ILE	3.0
35	1d	110	PHE	3.0
42	2k	95	ILE	3.0
47	1p	19	ILE	3.0
36	2e	99	GLY	3.0
41	2j	10	GLY	3.0
54	1w	17	G	3.0
34	2c	100	ALA	3.0
44	2m	91	ARG	3.0
12	2Q	103	MET	3.0
1	1A	1094	U	3.0

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Mol	Chain	Res	Type	RSRZ
11	2P	91	PHE	3.0
51	1t	9	ASN	3.0
6	2G	138	GLN	3.0
40	2i	113	LYS	3.0
54	1w	42	C	3.0
36	2e	84	PHE	3.0
41	2j	98	ILE	3.0
1	2A	6	A	3.0
1	2A	652(B)	A	3.0
36	2e	9	LYS	3.0
38	1g	85	TYR	3.0
49	2r	87	ARG	3.0
52	2u	9	ARG	3.0
6	2G	17	PRO	3.0
33	2b	48	MET	3.0
33	2b	94	ASN	3.0
42	2k	86	GLY	3.0
32	1a	1027	C	3.0
6	2G	141	PHE	3.0
38	1g	154	TYR	3.0
39	2h	94	TYR	3.0
44	2m	73	GLU	3.0
54	2w	37	A	3.0
20	2Y	42	VAL	3.0
44	2m	53	VAL	3.0
50	2s	36	ARG	3.0
32	1a	1023	G	3.0
6	2G	150	ASP	3.0
1	2A	2137	C	3.0
41	2j	56	HIS	3.0
42	2k	125	PHE	3.0
48	2q	27	PHE	3.0
52	1u	13	ILE	3.0
40	1i	112	LYS	3.0
56	2y	44	A	3.0
6	2G	37	VAL	2.9
35	1d	112	VAL	2.9
42	1k	92	GLU	2.9
33	1b	19	HIS	2.9
11	2P	75	ILE	2.9
39	1h	134	ILE	2.9
54	1w	73	U	2.9

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Mol	Chain	Res	Type	RSRZ
1	2A	886	C	2.9
50	2s	4	SER	2.9
38	1g	4	ARG	2.9
6	2G	2	PRO	2.9
8	2I	38	LEU	2.9
42	2k	75	TYR	2.9
4	2E	150	VAL	2.9
17	2V	5	VAL	2.9
35	1d	170	VAL	2.9
26	24	42	PHE	2.9
35	2d	158	ILE	2.9
39	2h	83	ILE	2.9
26	24	18	CYS	2.9
36	2e	14	ARG	2.9
1	2A	2153	G	2.9
32	2a	1021	G	2.9
38	2g	16	LEU	2.9
42	1k	75	TYR	2.9
43	2l	98	TYR	2.9
40	2i	28	VAL	2.9
42	2k	109	VAL	2.9
29	27	23	ARG	2.9
34	2c	162	GLN	2.9
34	2c	190	ARG	2.9
48	2q	59	ILE	2.9
33	2b	186	ALA	2.9
34	2c	71	ALA	2.9
41	2j	20	ALA	2.9
51	1t	20	LEU	2.9
56	1y	69	C	2.9
43	2l	69	TYR	2.9
1	1A	2151	G	2.9
32	1a	1002	G	2.9
7	2H	132	ARG	2.9
33	2b	209	ARG	2.9
38	2g	41	ARG	2.9
31	29	17	ILE	2.9
40	1i	33	PHE	2.9
47	2p	9	PHE	2.9
33	2b	51	LEU	2.9
34	2c	113	ALA	2.9
42	2k	98	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	1A	2164	C	2.9
34	1c	193	TYR	2.9
44	2m	99	ARG	2.9
48	2q	91	ARG	2.9
11	2P	83	VAL	2.9
21	2Z	126	VAL	2.9
30	28	16	ILE	2.9
32	2a	1286	A	2.9
33	2b	162	ILE	2.9
36	1e	6	PHE	2.9
54	2w	45	U	2.9
34	2c	18	TRP	2.9
44	2m	97	PRO	2.9
51	2t	59	ALA	2.9
33	2b	95	GLN	2.9
6	1G	146	TYR	2.9
6	2G	146	TYR	2.9
33	2b	8	LYS	2.9
45	2n	4	LYS	2.9
33	2b	89	GLY	2.9
40	2i	30	GLY	2.9
41	1j	50	ILE	2.9
34	2c	7	PRO	2.9
35	2d	49	ARG	2.9
56	1y	58	A	2.9
3	2D	182	LEU	2.9
1	2A	2108	C	2.8
8	2I	1	MET	2.8
50	2s	45	VAL	2.8
34	2c	77	ILE	2.8
54	2w	33	U	2.8
40	2i	116	LYS	2.8
1	1A	2125	G	2.8
33	2b	120	ALA	2.8
1	2A	896	A	2.8
40	2i	103	THR	2.8
48	2q	98	LEU	2.8
21	2Z	122	ARG	2.8
22	20	73	GLY	2.8
35	1d	122	ARG	2.8
35	1d	208	SER	2.8
47	1p	2	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
12	2Q	47	ILE	2.8
21	1Z	104	PHE	2.8
7	2H	20	ALA	2.8
39	2h	28	ALA	2.8
9	2N	116	LEU	2.8
33	2b	149	LEU	2.8
39	2h	10	LEU	2.8
38	2g	76	ARG	2.8
51	1t	22	ARG	2.8
51	1t	83	ARG	2.8
51	2t	26	ASN	2.8
47	1p	20	VAL	2.8
7	2H	29	PRO	2.8
17	2V	50	PRO	2.8
36	2e	8	GLU	2.8
48	2q	36	ILE	2.8
50	2s	75	ALA	2.8
9	2N	23	LEU	2.8
33	2b	205	ASP	2.8
32	2a	969	A	2.8
32	2a	1030(D)	A	2.8
32	2a	1092	A	2.8
32	2a	1492	A	2.8
35	2d	160	GLN	2.8
54	2w	9	A	2.8
7	2H	124	GLU	2.8
44	2m	98	VAL	2.8
26	24	67	TYR	2.8
38	2g	42	ILE	2.8
38	2g	62	PHE	2.8
50	2s	39	THR	2.8
55	2x	16	C	2.8
6	1G	139	LEU	2.8
35	1d	120	LEU	2.8
33	2b	72	GLY	2.8
34	2c	28	GLN	2.8
7	2H	125	VAL	2.8
21	2Z	100	VAL	2.8
32	1a	1030(D)	A	2.8
54	1w	27	A	2.8
54	1w	29	A	2.8
54	2w	44	A	2.8

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Mol	Chain	Res	Type	RSRZ
56	2y	9	A	2.8
7	2H	101	ARG	2.8
18	2W	92	ARG	2.8
1	2A	2132	U	2.8
3	2D	270	ILE	2.8
12	2Q	64	ILE	2.8
34	1c	189	ALA	2.8
40	2i	64	THR	2.8
41	2j	52	GLY	2.8
51	2t	20	LEU	2.8
6	2G	149	VAL	2.8
7	2H	128	PRO	2.8
43	2l	5	PRO	2.8
45	2n	33	VAL	2.8
32	2a	1250	A	2.8
54	1w	50	A	2.8
1	1A	2167	U	2.8
33	1b	228	GLY	2.8
33	2b	218	ALA	2.8
34	2c	200	ALA	2.8
35	1d	69	GLY	2.8
41	1j	98	ILE	2.8
42	1k	97	ALA	2.8
51	1t	32	ALA	2.8
1	2A	2190	G	2.8
1	2A	2894	G	2.8
4	2E	195	LEU	2.8
48	2q	37	LYS	2.8
1	2A	2896	C	2.8
44	2m	88	ARG	2.8
50	2s	51	VAL	2.7
1	1A	2189	U	2.7
2	2B	58	A	2.7
21	2Z	8	TYR	2.7
47	2p	48	TRP	2.7
21	1Z	120	ILE	2.7
26	24	44	THR	2.7
34	1c	182	ILE	2.7
34	2c	15	THR	2.7
48	2q	90	ILE	2.7
6	2G	173	LEU	2.7
29	17	47	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
44	2m	71	ARG	2.7
1	1A	2136	C	2.7
40	2i	75	ASP	2.7
40	2i	117	HIS	2.7
27	15	60	VAL	2.7
48	2q	87	LYS	2.7
43	1l	63	GLY	2.7
6	2G	100	TRP	2.7
28	26	54	ILE	2.7
35	1d	158	ILE	2.7
38	2g	115	ARG	2.7
40	2i	120	ARG	2.7
47	1p	36	ILE	2.7
50	2s	61	TYR	2.7
50	1s	15	LEU	2.7
56	1y	15	A	2.7
7	2H	111	HIS	2.7
39	1h	5	PRO	2.7
53	2v	19	G	2.7
26	24	10	VAL	2.7
31	29	16	VAL	2.7
34	2c	103	VAL	2.7
40	1i	41	VAL	2.7
42	2k	14	VAL	2.7
42	2k	80	VAL	2.7
48	2q	80	GLY	2.7
6	2G	151	ALA	2.7
39	2h	134	ILE	2.7
41	2j	50	ILE	2.7
6	2G	19	LEU	2.7
23	11	98	LEU	2.7
41	1j	8	LEU	2.7
48	1q	31	LEU	2.7
1	1A	278	A	2.7
1	2A	2126	A	2.7
44	1m	120	LYS	2.7
54	1w	37	A	2.7
33	2b	101	MET	2.7
1	2A	2103	C	2.7
42	2k	126	ARG	2.7
54	2w	62	C	2.7
56	1y	40	C	2.7

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Mol	Chain	Res	Type	RSRZ
19	2X	43	VAL	2.7
40	1i	109	VAL	2.7
48	2q	23	VAL	2.7
49	1r	39	VAL	2.7
1	1A	2182	G	2.7
1	1A	1065	U	2.7
54	1w	11	U	2.7
6	1G	152	LEU	2.7
33	2b	17	PHE	2.7
34	1c	134	ILE	2.7
47	1p	49	LEU	2.7
2	2B	59	A	2.7
34	2c	109	PRO	2.7
40	1i	51	ARG	2.7
43	2l	25	PRO	2.7
50	2s	76	PRO	2.7
55	2x	72	A	2.7
44	2m	13	LYS	2.7
50	2s	58	VAL	2.7
21	2Z	50	GLN	2.7
1	2A	9	U	2.7
17	2V	73	SER	2.7
56	1y	65	U	2.7
1	1A	2121	G	2.7
1	2A	2152	G	2.7
39	1h	2	LEU	2.7
49	2r	26	LEU	2.7
39	1h	58	TYR	2.7
40	2i	88	TYR	2.7
9	2N	74	ARG	2.7
21	1Z	119	GLU	2.7
51	2t	38	LYS	2.7
40	2i	91	ASP	2.7
6	2G	160	VAL	2.7
1	2A	1509	C	2.7
10	2O	41	ALA	2.7
35	1d	117	ALA	2.7
45	2n	8	GLU	2.7
6	2G	77	ILE	2.7
12	2Q	120	ILE	2.7
25	23	53	LEU	2.7
33	2b	223	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
38	2g	149	ARG	2.7
51	1t	62	LEU	2.7
54	1w	65	U	2.7
35	1d	23	GLY	2.7
54	1w	51	G	2.7
47	1p	48	TRP	2.7
41	2j	34	VAL	2.6
43	2l	55	VAL	2.6
3	1D	276	LYS	2.6
35	1d	166	LYS	2.6
32	1a	163	C	2.6
36	2e	130	ASN	2.6
40	2i	72	GLY	2.6
1	1A	2792	G	2.6
38	2g	119	ARG	2.6
1	2A	1847	A	2.6
21	1Z	164	ALA	2.6
32	1a	1001	A	2.6
12	2Q	34	LEU	2.6
54	1w	41	U	2.6
54	2w	59	U	2.6
56	1y	11	U	2.6
7	2H	159	GLU	2.6
32	1a	1037	C	2.6
34	2c	201	TYR	2.6
6	2G	8	LYS	2.6
26	14	55	ARG	2.6
1	2A	614(B)	G	2.6
45	2n	60	SER	2.6
7	2H	37	VAL	2.6
33	2b	197	VAL	2.6
6	2G	161	THR	2.6
26	14	19	GLY	2.6
26	14	57	GLU	2.6
45	1n	39	LEU	2.6
21	2Z	146	ILE	2.6
33	1b	17	PHE	2.6
33	2b	41	ILE	2.6
34	2c	39	ILE	2.6
46	1o	36	ILE	2.6
39	2h	135	CYS	2.6
52	1u	10	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	2A	897	C	2.6
32	2a	1028	C	2.6
54	1w	68	C	2.6
22	20	68	GLU	2.6
3	2D	18	VAL	2.6
33	2b	229	VAL	2.6
34	1c	148	GLY	2.6
43	2l	43	VAL	2.6
6	2G	103	LEU	2.6
30	28	15	LYS	2.6
32	1a	1033	G	2.6
33	1b	118	LEU	2.6
47	1p	27	LYS	2.6
21	2Z	124	ILE	2.6
35	1d	73	ARG	2.6
38	2g	88	PRO	2.6
32	2a	91	C	2.6
54	2w	68	C	2.6
54	2w	75	C	2.6
56	1y	61	C	2.6
34	1c	80	GLY	2.6
4	2E	196	VAL	2.6
21	1Z	141	VAL	2.6
39	2h	137	VAL	2.6
41	2j	46	ARG	2.6
41	2j	58	ASP	2.6
42	1k	14	VAL	2.6
44	2m	75	ALA	2.6
1	1A	2180	U	2.6
21	2Z	125	LEU	2.6
21	2Z	150	LEU	2.6
21	2Z	167	PRO	2.6
43	1l	27	LEU	2.6
46	1o	57	LEU	2.6
1	2A	2310	A	2.6
32	2a	1157	A	2.6
1	1A	2175	C	2.6
34	2c	145	GLY	2.6
45	2n	32	SER	2.6
7	2H	95	ARG	2.6
35	1d	102	ASP	2.6
41	2j	27	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
30	28	2	PRO	2.6
39	2h	119	LEU	2.6
51	1t	36	LEU	2.6
33	1b	211	ILE	2.6
43	1l	23	LYS	2.6
6	2G	95	ARG	2.6
20	2Y	50	ARG	2.6
31	29	19	ARG	2.6
11	2P	110	TYR	2.6
14	2S	92	TYR	2.6
1	1A	885	C	2.6
1	2A	2178	C	2.6
36	1e	21	ALA	2.5
40	2i	15	ALA	2.5
12	2Q	97	VAL	2.5
12	2Q	109	VAL	2.5
35	1d	78	LEU	2.5
46	2o	70	LEU	2.5
32	2a	1150	U	2.5
54	1w	45	U	2.5
40	1i	37	PHE	2.5
45	2n	7	ILE	2.5
51	2t	63	ILE	2.5
48	2q	75	ARG	2.5
33	1b	227	GLY	2.5
33	2b	220	ASP	2.5
1	2A	2125	G	2.5
32	2a	973	G	2.5
52	1u	18	TYR	2.5
7	2H	114	VAL	2.5
23	2l	53	VAL	2.5
36	1e	90	VAL	2.5
40	2i	79	LEU	2.5
51	2t	24	LEU	2.5
1	1A	2897	U	2.5
7	2H	72	ILE	2.5
36	1e	89	ILE	2.5
6	2G	48	GLU	2.5
34	2c	183	ASP	2.5
38	2g	34	GLY	2.5
34	2c	142	MET	2.5
47	1p	1	MET	2.5

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Mol	Chain	Res	Type	RSRZ
29	17	48	LYS	2.5
44	2m	76	ALA	2.5
6	2G	15	VAL	2.5
19	2X	65	ARG	2.5
20	2Y	45	VAL	2.5
36	2e	55	VAL	2.5
38	2g	3	ARG	2.5
44	2m	67	GLU	2.5
6	2G	49	ASP	2.5
34	1c	72	LYS	2.5
43	2l	7	ILE	2.5
52	2u	2	GLY	2.5
36	2e	10	MET	2.5
7	2H	165	ALA	2.5
12	2Q	59	ARG	2.5
38	2g	10	ARG	2.5
39	2h	122	ARG	2.5
38	2g	14	PRO	2.5
41	1j	97	GLU	2.5
43	2l	16	GLU	2.5
43	2l	65	GLU	2.5
1	2A	2171	A	2.5
23	2l	98	LEU	2.5
47	2p	20	VAL	2.5
51	1t	13	LEU	2.5
34	2c	78	GLY	2.5
54	2w	34	C	2.5
12	2Q	65	PHE	2.5
30	28	41	ILE	2.5
34	2c	10	PHE	2.5
34	2c	14	ILE	2.5
39	2h	31	PHE	2.5
9	2N	118	LYS	2.5
33	1b	133	LYS	2.5
49	2r	24	ALA	2.5
21	2Z	140	ASP	2.5
3	2D	3	VAL	2.5
23	2l	30	VAL	2.5
26	24	35	VAL	2.5
30	28	60	LEU	2.5
36	2e	34	VAL	2.5
40	1i	28	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
43	2l	93	LEU	2.5
46	1o	69	TYR	2.5
14	2S	40	ILE	2.5
21	2Z	137	ILE	2.5
34	1c	57	ILE	2.5
39	2h	111	ILE	2.5
3	2D	217	ARG	2.5
41	2j	51	ARG	2.5
42	2k	96	ARG	2.5
1	1A	2116	G	2.5
1	1A	2148	G	2.5
32	1a	1024	G	2.5
32	2a	1356	G	2.5
35	2d	161	ASN	2.5
38	2g	84	ASN	2.5
42	2k	90	GLY	2.5
50	2s	26	GLY	2.5
47	2p	6	LEU	2.5
49	2r	86	VAL	2.5
1	1A	1026	U	2.5
25	23	30	ARG	2.5
40	2i	83	ARG	2.5
35	1d	181	MET	2.5
1	1A	1176	G	2.5
1	1A	2101	G	2.5
40	2i	43	ALA	2.5
6	2G	35	GLU	2.5
7	2H	135	GLY	2.5
33	2b	177	ALA	2.5
51	1t	73	HIS	2.4
8	2I	12	LEU	2.4
12	2Q	102	VAL	2.4
34	1c	55	VAL	2.4
47	2p	39	TYR	2.4
32	2a	1358	U	2.4
4	2E	51	PHE	2.4
1	1A	2178	C	2.4
43	2l	8	ASN	2.4
51	2t	9	ASN	2.4
43	2l	46	LYS	2.4
50	2s	69	HIS	2.4
34	1c	12	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
51	2t	62	LEU	2.4
21	2Z	99	TYR	2.4
9	2N	85	ILE	2.4
45	2n	46	GLU	2.4
6	2G	47	LYS	2.4
33	2b	38	GLY	2.4
32	1a	1531	A	2.4
41	1j	21	GLN	2.4
56	1y	44	A	2.4
33	2b	188	ALA	2.4
40	1i	15	ALA	2.4
45	2n	49	HIS	2.4
33	2b	145	LEU	2.4
34	2c	188	LEU	2.4
38	2g	104	LEU	2.4
43	2l	10	LEU	2.4
51	1t	72	LEU	2.4
6	2G	159	VAL	2.4
35	1d	207	TYR	2.4
54	2w	51	G	2.4
55	2x	70	G	2.4
3	2D	64	ILE	2.4
33	2b	185	ILE	2.4
34	2c	57	ILE	2.4
26	24	48	ARG	2.4
7	2H	34	GLU	2.4
32	2a	1363(A)	A	2.4
8	2I	31	LEU	2.4
34	2c	20	SER	2.4
44	2m	96	LEU	2.4
51	2t	13	LEU	2.4
8	2I	3	VAL	2.4
45	1n	25	VAL	2.4
12	2Q	6	ARG	2.4
48	2q	92	ARG	2.4
1	1A	2154	G	2.4
42	2k	69	ALA	2.4
33	1b	124	SER	2.4
35	2d	19	LEU	2.4
54	1w	40	C	2.4
54	2w	6	C	2.4
14	2S	14	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
14	2S	46	VAL	2.4
35	1d	8	VAL	2.4
47	2p	38	TYR	2.4
41	2j	13	HIS	2.4
22	20	10	THR	2.4
50	2s	77	THR	2.4
7	2H	84	SER	2.4
37	2f	45	LEU	2.4
38	2g	99	LEU	2.4
18	2W	20	VAL	2.4
42	2k	17	GLY	2.4
44	1m	117	VAL	2.4
48	2q	73	VAL	2.4
20	1Y	1	MET	2.4
40	1i	114	TYR	2.4
9	2N	102	ALA	2.4
10	2O	51	ALA	2.4
47	2p	64	ALA	2.4
39	1h	3	THR	2.4
1	1A	2100	G	2.3
1	1A	2157	G	2.3
32	1a	1032	G	2.3
6	2G	154	GLY	2.3
23	21	29	GLY	2.3
25	23	54	VAL	2.3
38	2g	135	VAL	2.3
1	1A	886	C	2.3
21	2Z	121	HIS	2.3
34	2c	174	PRO	2.3
22	20	55	ARG	2.3
38	2g	31	MET	2.3
43	2l	100	ILE	2.3
33	1b	70	PHE	2.3
33	1b	226	ARG	2.3
48	2q	38	ARG	2.3
3	1D	2	ALA	2.3
6	1G	73	ALA	2.3
9	2N	83	LYS	2.3
6	2G	133	LEU	2.3
21	2Z	163	LEU	2.3
35	2d	162	LEU	2.3
1	2A	2106	G	2.3

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Mol	Chain	Res	Type	RSRZ
8	2I	107	VAL	2.3
1	2A	2130	U	2.3
9	2N	108	PRO	2.3
43	2I	41	ARG	2.3
1	1A	1057	A	2.3
1	1A	2135	A	2.3
26	24	31	ILE	2.3
41	1j	4	ILE	2.3
41	2j	61	GLU	2.3
54	1w	15	A	2.3
55	2x	69	C	2.3
44	1m	87	TYR	2.3
44	2m	43	THR	2.3
11	2P	93	GLY	2.3
40	1i	117	HIS	2.3
35	1d	104	VAL	2.3
36	2e	67	VAL	2.3
32	2a	1196	U	2.3
42	2k	39	PRO	2.3
45	2n	56	VAL	2.3
1	1A	2805	G	2.3
55	2x	71	C	2.3
1	1A	887	A	2.3
12	2Q	28	ALA	2.3
38	2g	152	ALA	2.3
52	1u	21	TYR	2.3
12	2Q	86	GLY	2.3
5	2F	123	LEU	2.3
6	2G	135	LEU	2.3
11	2P	105	LEU	2.3
17	2V	71	LEU	2.3
33	2b	215	LEU	2.3
3	2D	275	LYS	2.3
14	2S	11	LYS	2.3
36	1e	96	PRO	2.3
1	1A	1081	U	2.3
1	1A	2122	U	2.3
32	2a	961	U	2.3
53	1v	22	U	2.3
54	2w	12	U	2.3
4	2E	77	ILE	2.3
10	2O	19	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
17	2V	70	ILE	2.3
1	2A	894	C	2.3
6	2G	137	GLU	2.3
8	2I	49	ALA	2.3
19	2X	60	ARG	2.3
32	2a	1452	C	2.3
34	2c	163	ALA	2.3
36	2e	16	THR	2.3
38	2g	8	GLU	2.3
41	1j	46	ARG	2.3
54	2w	66	C	2.3
1	1A	2801(A)	A	2.3
1	2A	2151	G	2.3
16	2U	60	LEU	2.3
40	1i	50	LEU	2.3
43	2l	48	PRO	2.3
5	1F	89	VAL	2.3
34	2c	153	VAL	2.3
40	1i	65	VAL	2.3
1	2A	614(A)	U	2.3
12	2Q	15	GLY	2.3
42	2k	108	ILE	2.3
1	2A	2163	C	2.3
18	2W	86	LEU	2.3
39	1h	112	LEU	2.3
1	2A	2157	G	2.3
32	2a	1108	G	2.3
54	1w	58	A	2.3
6	2G	112	PRO	2.3
25	23	16	PRO	2.3
8	2I	85	GLU	2.3
7	2H	45	VAL	2.3
26	24	55	ARG	2.3
28	26	52	VAL	2.3
36	2e	33	VAL	2.3
56	1y	43	U	2.3
22	20	52	GLY	2.3
42	1k	90	GLY	2.3
16	2U	40	PHE	2.3
35	1d	147	ALA	2.3
38	2g	13	GLN	2.3
33	2b	140	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
45	2n	27	CYS	2.3
1	2A	1816	G	2.2
54	1w	22	G	2.2
16	2U	9	VAL	2.2
35	1d	167	GLY	2.2
50	2s	9	VAL	2.2
44	2m	105	THR	2.2
3	2D	155	LEU	2.2
6	1G	136	ARG	2.2
6	2G	62	LEU	2.2
7	2H	6	ARG	2.2
21	2Z	5	LEU	2.2
33	2b	115	LEU	2.2
37	2f	21	LEU	2.2
38	1g	16	LEU	2.2
39	1h	133	LEU	2.2
47	1p	6	LEU	2.2
49	1r	85	LEU	2.2
39	2h	65	TYR	2.2
6	2G	27	ASN	2.2
9	2N	69	GLN	2.2
30	28	22	VAL	2.2
32	2a	965	A	2.2
32	2a	975	A	2.2
38	2g	33	ASP	2.2
48	1q	57	VAL	2.2
1	1A	1087	G	2.2
1	2A	1170	G	2.2
1	2A	2131	G	2.2
32	2a	1024	G	2.2
34	2c	105	GLU	2.2
54	1w	18	G	2.2
6	2G	73	ALA	2.2
22	20	69	PHE	2.2
36	1e	138	ALA	2.2
45	1n	59	ALA	2.2
45	2n	15	LYS	2.2
51	1t	74	LYS	2.2
38	1g	78	ARG	2.2
38	2g	94	ARG	2.2
44	2m	100	GLY	2.2
1	1A	2177	C	2.2

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Mol	Chain	Res	Type	RSRZ
32	2a	1066	C	2.2
32	2a	1234	C	2.2
20	2Y	81	LYS	2.2
42	2k	84	VAL	2.2
43	1l	55	VAL	2.2
54	2w	46	A	2.2
6	2G	153	ARG	2.2
12	2Q	114	ALA	2.2
23	2l	13	ILE	2.2
51	1t	33	ILE	2.2
51	2t	17	ARG	2.2
35	1d	206	PHE	2.2
5	2F	33	LEU	2.2
48	2q	22	LEU	2.2
3	2D	236	GLY	2.2
8	2I	29	TYR	2.2
8	2I	82	ARG	2.2
12	2Q	5	ARG	2.2
12	2Q	35	VAL	2.2
32	2a	1116	C	2.2
36	1e	136	MET	2.2
52	1u	9	ARG	2.2
54	1w	12	U	2.2
32	1a	161	A	2.2
45	2n	30	ALA	2.2
9	2N	45	ASN	2.2
35	2d	167	GLY	2.2
41	1j	90	LEU	2.2
7	2H	157	TYR	2.2
35	1d	65	ARG	2.2
42	1k	42	TRP	2.2
45	2n	21	TYR	2.2
38	2g	66	VAL	2.2
48	2q	77	VAL	2.2
21	1Z	169	GLU	2.2
21	1Z	146	ILE	2.2
14	2S	87	PHE	2.2
22	20	45	PHE	2.2
32	2a	1493	A	2.2
33	1b	163	PHE	2.2
35	1d	75	PHE	2.2
43	2l	49	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
54	1w	44	A	2.2
11	2P	78	PRO	2.2
19	2X	95	LEU	2.2
28	26	13	CYS	2.2
45	2n	54	PRO	2.2
48	1q	28	PRO	2.2
34	2c	172	ARG	2.2
10	2O	7	TYR	2.2
21	2Z	162	GLU	2.2
50	1s	38	SER	2.2
7	2H	169	VAL	2.2
9	2N	46	VAL	2.2
36	1e	69	VAL	2.2
45	1n	56	VAL	2.2
6	2G	110	ALA	2.2
43	2l	51	ALA	2.2
49	1r	73	ALA	2.2
7	2H	121	ILE	2.2
35	1d	5	ILE	2.2
44	2m	26	GLY	2.2
25	23	12	PRO	2.2
33	1b	125	PRO	2.2
34	1c	190	ARG	2.2
34	2c	59	ARG	2.2
8	2I	9	LEU	2.2
36	2e	31	LEU	2.2
44	2m	81	LEU	2.2
45	2n	47	LEU	2.2
46	1o	56	LEU	2.2
46	2o	66	LEU	2.2
33	2b	147	LYS	2.1
1	2A	892	G	2.1
32	2a	1068	G	2.1
33	2b	219	VAL	2.1
43	1l	39	VAL	2.1
42	1k	15	ALA	2.1
42	1k	89	ALA	2.1
35	2d	122	ARG	2.1
51	2t	22	ARG	2.1
33	1b	80	ILE	2.1
34	1c	15	THR	2.1
1	1A	897	C	2.1

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Mol	Chain	Res	Type	RSRZ
20	2Y	60	PHE	2.1
32	2a	980	C	2.1
33	2b	143	GLU	2.1
36	2e	45	PHE	2.1
49	2r	46	GLU	2.1
3	2D	206	LEU	2.1
26	24	9	LEU	2.1
39	1h	10	LEU	2.1
46	2o	56	LEU	2.1
48	2q	6	LEU	2.1
31	29	13	LYS	2.1
48	2q	100	LYS	2.1
25	23	11	SER	2.1
34	1c	179	ARG	2.1
35	1d	38	TYR	2.1
7	2H	99	VAL	2.1
35	1d	198	VAL	2.1
42	1k	84	VAL	2.1
51	1t	80	ARG	2.1
6	2G	164	GLU	2.1
7	2H	78	GLY	2.1
25	23	51	ALA	2.1
38	1g	34	GLY	2.1
42	2k	42	TRP	2.1
51	1t	40	ALA	2.1
26	24	29	PRO	2.1
32	2a	1002	G	2.1
35	1d	204	ILE	2.1
55	2x	2	G	2.1
7	2H	71	LEU	2.1
13	2R	65	LEU	2.1
34	1c	91	LEU	2.1
55	1x	1	C	2.1
9	2N	101	HIS	2.1
35	2d	47	ARG	2.1
44	2m	93	ARG	2.1
7	2H	47	GLU	2.1
32	2a	983	A	2.1
32	2a	1225	A	2.1
4	2E	115	GLY	2.1
36	2e	85	GLY	2.1
1	1A	1060	U	2.1

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Mol	Chain	Res	Type	RSRZ
7	2H	17	VAL	2.1
11	2P	39	LYS	2.1
34	2c	2	GLY	2.1
35	1d	2	GLY	2.1
22	20	63	VAL	2.1
32	1a	202	U	2.1
34	2c	53	ALA	2.1
40	2i	53	VAL	2.1
52	2u	18	TYR	2.1
33	1b	95	GLN	2.1
36	2e	131	ILE	2.1
39	2h	86	ILE	2.1
6	2G	117	PHE	2.1
19	1X	95	LEU	2.1
29	27	41	ARG	2.1
32	2a	951	G	2.1
1	2A	2177	C	2.1
32	2a	1397	C	2.1
50	2s	3	ARG	2.1
11	2P	28	GLY	2.1
1	1A	1847	A	2.1
32	2a	1111	A	2.1
54	1w	21	A	2.1
11	2P	31	ALA	2.1
30	28	23	VAL	2.1
34	1c	23	TYR	2.1
34	1c	198	VAL	2.1
35	2d	121	VAL	2.1
36	2e	17	ALA	2.1
37	2f	9	VAL	2.1
38	2g	39	ALA	2.1
47	1p	39	TYR	2.1
7	2H	12	PRO	2.1
38	1g	120	ILE	2.1
42	2k	21	ILE	2.1
14	2S	12	PHE	2.1
31	29	9	ARG	2.1
33	1b	187	LEU	2.1
33	2b	231	GLU	2.1
34	1c	47	LEU	2.1
34	2c	21	ARG	2.1
34	2c	22	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
35	1d	168	ARG	2.1
35	1d	202	LEU	2.1
51	1t	24	LEU	2.1
3	2D	202	LYS	2.1
42	2k	107	SER	2.1
32	2a	1007	C	2.1
32	2a	1221	G	2.1
51	1t	18	GLN	2.1
36	2e	21	ALA	2.1
43	1l	26	ALA	2.1
46	2o	16	ALA	2.1
51	1t	67	ALA	2.1
1	1A	896	A	2.1
10	2O	52	VAL	2.1
20	2Y	24	VAL	2.1
33	1b	77	ALA	2.1
11	2P	149	GLU	2.1
33	2b	31	TYR	2.1
37	2f	59	TYR	2.1
44	1m	103	THR	2.1
48	2q	86	GLU	2.1
51	2t	25	ARG	2.1
14	2S	57	LYS	2.1
21	2Z	154	ASP	2.1
33	1b	200	ILE	2.1
44	1m	121	LYS	2.1
7	2H	88	LEU	2.1
33	1b	233	SER	2.1
35	1d	108	LEU	2.1
35	2d	157	LEU	2.1
49	2r	78	LEU	2.1
51	2t	72	LEU	2.1
22	20	12	ASN	2.1
50	2s	65	ASN	2.1
12	2Q	33	GLY	2.1
19	1X	94	GLY	2.1
26	24	53	GLU	2.1
11	2P	76	LYS	2.1
11	2P	90	ARG	2.1
34	2c	199	LYS	2.1
51	1t	68	LYS	2.1
21	1Z	165	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
21	1Z	170	THR	2.1
39	1h	93	VAL	2.1
42	2k	114	VAL	2.1
26	24	25	TYR	2.1
36	2e	133	TYR	2.1
33	2b	39	ILE	2.1
41	2j	75	ILE	2.1
41	2j	96	ILE	2.1
50	2s	83	HIS	2.1
55	2x	73	A	2.1
36	2e	125	SER	2.1
41	2j	11	PHE	2.1
43	2l	62	SER	2.1
11	2P	68	GLN	2.1
34	1c	2	GLY	2.1
47	1p	37	GLY	2.1
52	1u	14	TRP	2.1
6	2G	181	ARG	2.1
33	2b	74	LYS	2.1
51	1t	14	LYS	2.1
1	2A	2107	C	2.0
6	2G	32	PRO	2.0
20	2Y	65	ALA	2.0
21	1Z	51	ALA	2.0
34	1c	60	ALA	2.0
34	2c	191	THR	2.0
42	1k	82	VAL	2.0
1	1A	1059	G	2.0
40	2i	4	TYR	2.0
56	1y	17	G	2.0
9	2N	26	LEU	2.0
11	2P	6	LEU	2.0
6	2G	42	GLY	2.0
32	1a	344	A	2.0
35	1d	185	PHE	2.0
38	2g	139	GLU	2.0
40	2i	87	GLN	2.0
48	1q	6	LEU	2.0
16	2U	16	LYS	2.0
39	2h	84	ARG	2.0
40	2i	16	ARG	2.0
51	1t	89	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
39	2h	9	MET	2.0
23	2l	68	PRO	2.0
33	1b	188	ALA	2.0
33	2b	159	PRO	2.0
32	2a	1326	C	2.0
43	2l	36	VAL	2.0
54	2w	63	C	2.0
51	2t	34	LYS	2.0
10	1O	50	GLY	2.0
12	2Q	37	LEU	2.0
22	20	65	GLY	2.0
33	2b	200	ILE	2.0
34	1c	14	ILE	2.0
49	2r	44	LEU	2.0
50	2s	22	LEU	2.0
1	1A	1068	G	2.0
22	20	60	PHE	2.0
29	27	18	PHE	2.0
40	2i	18	PHE	2.0
41	2j	89	ASP	2.0
6	2G	13	GLU	2.0
12	2Q	22	LYS	2.0
15	1T	35	LYS	2.0
34	2c	72	LYS	2.0
38	2g	100	ALA	2.0
40	1i	116	LYS	2.0
5	2F	89	VAL	2.0
30	18	14	VAL	2.0
35	1d	118	ARG	2.0
51	2t	83	ARG	2.0
1	2A	34	C	2.0
7	2H	166	GLY	2.0
35	2d	70	ILE	2.0
37	2f	48	LEU	2.0
33	1b	33	TYR	2.0
1	2A	2173	A	2.0
54	1w	46	A	2.0
35	1d	7	PRO	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	PSU	2y	55	20/21	0.55	0.56	93,99,107,111	0
56	4SU	2y	8	20/21	0.62	0.30	90,98,104,115	0
54	PSU	1w	55	20/21	0.63	0.46	81,89,98,101	0
54	PSU	2w	55	20/21	0.64	0.38	87,94,102,114	0
56	PSU	1y	55	20/21	0.69	0.43	88,93,98,104	0
56	5MU	1y	54	21/22	0.69	0.42	86,90,94,107	0
54	5MU	2w	54	21/22	0.73	0.26	83,91,97,101	0
56	5MU	2y	54	21/22	0.73	0.56	88,95,99,117	0
54	4SU	2w	8	20/21	0.75	0.39	89,95,110,110	0
56	4SU	1y	8	20/21	0.80	0.29	90,95,100,115	0
54	4SU	1w	8	20/21	0.84	0.21	87,93,103,113	0
54	5MU	1w	54	21/22	0.85	0.28	67,82,88,91	0
43	0TD	2l	92	10/11	0.86	0.18	67,71,78,82	0
32	2MG	2a	1207	24/25	0.87	0.19	81,85,92,101	0
55	4SU	2x	8	20/21	0.87	0.16	75,78,83,86	0
55	PSU	2x	55	20/21	0.88	0.17	73,78,87,92	0
1	5MU	2A	1915	21/22	0.89	0.15	74,78,82,92	0
55	5MU	2x	54	21/22	0.90	0.25	74,82,88,92	0
32	PSU	2a	516	20/21	0.91	0.15	73,79,84,84	0
43	0TD	1l	92	10/11	0.91	0.17	44,53,59,67	0
32	M2G	2a	966	25/26	0.92	0.23	62,68,83,90	0
32	4OC	2a	1402	22/23	0.92	0.20	52,66,68,73	0
32	5MC	2a	967	21/22	0.92	0.18	66,69,78,82	0
1	5MU	1A	1915	21/22	0.93	0.19	49,61,65,74	0
1	PSU	2A	1917	20/21	0.93	0.18	58,71,80,82	0
54	L3X	2w	76	26/27	0.93	0.35	45,57,62,63	0
55	PSU	1x	55	20/21	0.94	0.18	53,62,69,73	0
1	PSU	1A	1917	20/21	0.94	0.16	42,54,60,61	0
32	5MC	2a	1400	21/22	0.94	0.29	68,74,78,82	0
32	2MG	1a	1207	24/25	0.94	0.15	68,72,77,77	0
55	4SU	1x	8	20/21	0.94	0.18	51,61,66,67	0
32	5MC	2a	1404	21/22	0.94	0.21	54,60,69,71	0
55	5MU	1x	54	21/22	0.94	0.16	60,68,70,74	0
32	MA6	2a	1519	24/25	0.94	0.25	54,64,68,68	0
32	G7M	2a	527	24/25	0.95	0.15	67,70,74,82	0
55	31H	2x	76	32/33	0.95	0.27	46,53,59,61	0
32	PSU	1a	516	20/21	0.95	0.16	60,63,66,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	5MC	1a	967	21/22	0.95	0.22	49,54,59,60	0
55	5MC	2x	32	21/22	0.95	0.17	66,73,76,80	0
1	OMC	2A	1920	21/22	0.95	0.20	57,63,66,68	0
1	PSU	2A	1911	20/21	0.95	0.17	58,63,68,70	0
54	L3X	1w	76	26/27	0.95	0.22	31,42,47,48	0
55	5MC	1x	32	21/22	0.96	0.19	51,56,61,64	0
32	5MC	2a	1407	21/22	0.96	0.19	45,57,65,68	0
32	UR3	2a	1498	21/22	0.96	0.18	54,59,65,68	0
32	MA6	2a	1518	24/25	0.96	0.21	47,62,70,71	0
32	M2G	1a	966	25/26	0.96	0.19	44,52,60,65	0
1	PSU	2A	2605	20/21	0.96	0.21	35,40,45,46	0
55	31H	1x	76	32/33	0.96	0.22	21,31,39,51	10
1	OMG	2A	2251	24/25	0.97	0.22	37,42,44,51	0
1	OMU	2A	2552	21/22	0.97	0.19	32,39,42,47	0
32	MA6	1a	1519	24/25	0.97	0.18	35,40,44,46	0
1	5MC	1A	1942	21/22	0.97	0.21	31,41,46,55	0
1	PSU	1A	1911	20/21	0.97	0.18	39,47,52,52	0
32	G7M	1a	527	24/25	0.97	0.21	43,48,54,58	0
32	5MC	1a	1400	21/22	0.97	0.17	38,49,54,58	0
32	MA6	1a	1518	24/25	0.97	0.22	34,38,46,50	0
1	5MC	2A	1942	21/22	0.97	0.18	43,53,57,61	0
1	5MC	2A	1962	21/22	0.97	0.19	36,45,56,57	0
32	UR3	1a	1498	21/22	0.98	0.18	32,39,43,46	0
1	PSU	1A	2605	20/21	0.98	0.21	23,26,32,32	0
1	5MU	1A	1939	21/22	0.98	0.21	24,27,30,32	0
1	OMC	1A	1920	21/22	0.98	0.22	34,45,48,50	0
1	5MC	1A	1962	21/22	0.98	0.18	23,32,37,41	0
1	OMG	1A	2251	24/25	0.98	0.20	22,25,26,27	0
1	2MA	1A	2503	23/24	0.98	0.21	17,22,25,28	0
1	OMU	1A	2552	21/22	0.98	0.23	22,28,31,33	0
1	5MU	2A	1939	21/22	0.98	0.18	30,35,40,47	0
32	4OC	1a	1402	22/23	0.98	0.20	37,46,50,58	0
32	5MC	1a	1404	21/22	0.98	0.18	30,37,41,43	0
32	5MC	1a	1407	21/22	0.98	0.21	36,41,44,48	0
1	2MA	2A	2503	23/24	0.98	0.21	30,36,40,43	0

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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	MG	1A	4007	1/1	-0.16	0.15	82,82,82,82	0
57	MG	2a	1605	1/1	0.34	0.22	73,73,73,73	0
57	MG	2a	1603	1/1	0.35	0.21	72,72,72,72	0
57	MG	1A	3101	1/1	0.38	0.12	74,74,74,74	0
57	MG	28	103	1/1	0.39	0.23	88,88,88,88	0
57	MG	1A	3517	1/1	0.43	0.25	57,57,57,57	0
57	MG	2a	1649	1/1	0.43	0.21	80,80,80,80	0
57	MG	1a	1633	1/1	0.44	0.21	69,69,69,69	0
57	MG	1A	3973	1/1	0.45	0.12	55,55,55,55	0
57	MG	1a	1767	1/1	0.45	0.16	60,60,60,60	0
57	MG	1a	1783	1/1	0.47	0.22	75,75,75,75	0
57	MG	2a	1642	1/1	0.48	0.17	62,62,62,62	0
57	MG	2A	3089	1/1	0.49	0.15	86,86,86,86	0
57	MG	1a	1668	1/1	0.49	0.28	65,65,65,65	0
57	MG	1w	108	1/1	0.49	0.15	64,64,64,64	0
57	MG	2A	3192	1/1	0.50	0.72	67,67,67,67	0
57	MG	1A	3801	1/1	0.50	0.10	74,74,74,74	0
57	MG	1A	4071	1/1	0.50	0.36	73,73,73,73	0
57	MG	2v	101	1/1	0.50	0.29	83,83,83,83	0
57	MG	1A	3732	1/1	0.51	0.31	62,62,62,62	0
57	MG	2A	3826	1/1	0.52	0.09	57,57,57,57	0
57	MG	2A	3804	1/1	0.54	0.11	69,69,69,69	0
57	MG	2A	3835	1/1	0.54	0.12	70,70,70,70	0
59	ZN	24	501	1/1	0.54	0.19	138,138,138,138	0
57	MG	1A	3882	1/1	0.55	0.17	47,47,47,47	0
57	MG	2x	105	1/1	0.55	0.20	75,75,75,75	0
57	MG	2A	3361	1/1	0.55	0.09	75,75,75,75	0
57	MG	2a	1707	1/1	0.56	0.21	76,76,76,76	0
57	MG	2A	3298	1/1	0.56	0.19	67,67,67,67	0
57	MG	2A	3224	1/1	0.57	0.22	57,57,57,57	0
57	MG	2A	3098	1/1	0.57	0.21	82,82,82,82	0
57	MG	1A	4043	1/1	0.57	0.13	56,56,56,56	0
57	MG	2A	3609	1/1	0.57	0.36	62,62,62,62	0
57	MG	1A	3079	1/1	0.58	0.23	53,53,53,53	0
57	MG	1A	4006	1/1	0.58	0.22	68,68,68,68	0
57	MG	2A	3255	1/1	0.58	0.35	62,62,62,62	0
57	MG	2A	3199	1/1	0.60	0.16	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1B	207	1/1	0.60	0.17	76,76,76,76	0
57	MG	1A	3480	1/1	0.61	0.26	68,68,68,68	0
57	MG	1a	1705	1/1	0.61	0.17	71,71,71,71	0
57	MG	1E	313	1/1	0.62	0.37	68,68,68,68	0
57	MG	2A	3328	1/1	0.62	0.15	80,80,80,80	0
57	MG	2a	1817	1/1	0.62	0.27	77,77,77,77	0
57	MG	2A	3662	1/1	0.62	0.15	68,68,68,68	0
57	MG	2a	1625	1/1	0.62	0.19	67,67,67,67	0
57	MG	2B	216	1/1	0.62	0.13	77,77,77,77	0
57	MG	1B	230	1/1	0.63	0.13	71,71,71,71	0
57	MG	1A	3248	1/1	0.63	0.22	66,66,66,66	0
57	MG	2A	3389	1/1	0.64	0.36	65,65,65,65	0
57	MG	1A	3765	1/1	0.64	0.19	61,61,61,61	0
57	MG	2a	1720	1/1	0.64	0.43	67,67,67,67	0
57	MG	2A	3362	1/1	0.64	0.15	70,70,70,70	0
57	MG	2A	3779	1/1	0.64	0.50	81,81,81,81	0
57	MG	2G	201	1/1	0.64	0.12	75,75,75,75	0
57	MG	2a	1644	1/1	0.64	0.17	70,70,70,70	0
57	MG	2A	3861	1/1	0.65	0.25	73,73,73,73	0
57	MG	1A	3984	1/1	0.65	0.16	67,67,67,67	0
57	MG	1A	4046	1/1	0.65	0.15	50,50,50,50	0
57	MG	1A	3618	1/1	0.65	0.27	65,65,65,65	0
57	MG	2a	1765	1/1	0.65	0.13	55,55,55,55	0
57	MG	2A	3193	1/1	0.65	0.14	63,63,63,63	0
57	MG	2A	3335	1/1	0.65	0.12	69,69,69,69	0
57	MG	2A	3198	1/1	0.65	0.29	69,69,69,69	0
57	MG	1A	3026	1/1	0.65	0.35	66,66,66,66	0
57	MG	1w	105	1/1	0.66	0.17	77,77,77,77	0
57	MG	1A	4021	1/1	0.66	0.34	63,63,63,63	0
57	MG	1A	3458	1/1	0.66	0.19	59,59,59,59	0
57	MG	2A	3350	1/1	0.66	0.20	70,70,70,70	0
57	MG	1D	311	1/1	0.66	0.16	77,77,77,77	0
57	MG	1a	1822	1/1	0.66	0.12	67,67,67,67	0
57	MG	2A	3281	1/1	0.67	0.12	67,67,67,67	0
57	MG	1x	107	1/1	0.67	0.20	63,63,63,63	0
57	MG	1A	3368	1/1	0.67	0.22	57,57,57,57	0
57	MG	2A	3379	1/1	0.67	0.82	64,64,64,64	0
57	MG	2A	3806	1/1	0.67	0.12	41,41,41,41	0
57	MG	1w	101	1/1	0.67	0.19	84,84,84,84	0
57	MG	1a	1738	1/1	0.68	0.10	76,76,76,76	0
57	MG	1B	234	1/1	0.68	0.19	75,75,75,75	0
57	MG	20	102	1/1	0.68	0.15	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3164	1/1	0.68	0.18	59,59,59,59	0
57	MG	1a	1809	1/1	0.68	0.15	71,71,71,71	0
57	MG	1A	3926	1/1	0.68	0.17	60,60,60,60	0
57	MG	2A	3423	1/1	0.68	0.14	84,84,84,84	0
57	MG	2A	3204	1/1	0.68	0.10	75,75,75,75	0
57	MG	1S	203	1/1	0.68	0.26	75,75,75,75	0
57	MG	2A	3734	1/1	0.68	0.17	72,72,72,72	0
57	MG	2A	3746	1/1	0.68	0.95	66,66,66,66	0
57	MG	1A	3806	1/1	0.68	0.13	39,39,39,39	0
57	MG	1B	226	1/1	0.68	0.16	65,65,65,65	0
57	MG	1A	3827	1/1	0.68	0.20	48,48,48,48	0
57	MG	2A	3318	1/1	0.68	1.08	62,62,62,62	0
57	MG	2A	3087	1/1	0.68	0.17	75,75,75,75	0
57	MG	1a	1721	1/1	0.68	0.17	63,63,63,63	0
57	MG	1a	1629	1/1	0.69	0.16	57,57,57,57	0
57	MG	2A	3008	1/1	0.69	0.18	61,61,61,61	0
57	MG	2A	3575	1/1	0.69	0.14	69,69,69,69	0
57	MG	1h	201	1/1	0.69	0.16	60,60,60,60	0
57	MG	1A	3500	1/1	0.69	0.17	55,55,55,55	0
57	MG	2A	3706	1/1	0.69	0.16	37,37,37,37	0
57	MG	1a	1806	1/1	0.69	0.20	64,64,64,64	0
57	MG	2A	3188	1/1	0.69	0.29	59,59,59,59	0
57	MG	2A	3269	1/1	0.69	0.26	72,72,72,72	0
57	MG	1A	4025	1/1	0.69	0.11	75,75,75,75	0
57	MG	2a	1614	1/1	0.69	0.15	78,78,78,78	0
57	MG	2A	3622	1/1	0.70	0.28	61,61,61,61	0
57	MG	1B	228	1/1	0.70	0.25	81,81,81,81	0
57	MG	2A	3488	1/1	0.70	0.23	58,58,58,58	0
57	MG	2A	3730	1/1	0.70	0.13	65,65,65,65	0
57	MG	2A	3054	1/1	0.70	0.26	70,70,70,70	0
57	MG	1A	3094	1/1	0.70	0.17	51,51,51,51	0
57	MG	2A	3268	1/1	0.71	0.27	75,75,75,75	0
57	MG	2a	1655	1/1	0.71	0.11	60,60,60,60	0
57	MG	2a	1662	1/1	0.71	0.15	67,67,67,67	0
57	MG	2a	1664	1/1	0.71	0.21	68,68,68,68	0
57	MG	2a	1705	1/1	0.71	0.21	77,77,77,77	0
57	MG	1A	3392	1/1	0.71	0.20	50,50,50,50	0
57	MG	1A	3370	1/1	0.71	0.15	51,51,51,51	0
57	MG	2A	3033	1/1	0.71	0.13	57,57,57,57	0
57	MG	1A	3666	1/1	0.71	0.14	63,63,63,63	0
57	MG	1a	1677	1/1	0.71	0.21	74,74,74,74	0
57	MG	2A	3333	1/1	0.71	0.16	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3334	1/1	0.71	0.14	73,73,73,73	0
57	MG	2A	3375	1/1	0.72	0.20	70,70,70,70	0
57	MG	1a	1727	1/1	0.72	0.27	61,61,61,61	0
57	MG	1A	4090	1/1	0.72	0.12	58,58,58,58	0
57	MG	1x	105	1/1	0.72	0.22	69,69,69,69	0
57	MG	2A	3323	1/1	0.72	0.27	74,74,74,74	0
57	MG	1a	1666	1/1	0.72	0.20	66,66,66,66	0
57	MG	2a	1672	1/1	0.72	0.24	72,72,72,72	0
57	MG	1A	3421	1/1	0.72	0.23	62,62,62,62	0
57	MG	1A	3438	1/1	0.72	0.17	60,60,60,60	0
57	MG	1a	1683	1/1	0.72	0.18	55,55,55,55	0
57	MG	2A	3679	1/1	0.72	0.09	61,61,61,61	0
57	MG	2A	3343	1/1	0.72	0.31	70,70,70,70	0
57	MG	1a	1692	1/1	0.72	0.16	70,70,70,70	0
57	MG	2x	102	1/1	0.72	0.13	75,75,75,75	0
57	MG	1A	3346	1/1	0.72	0.52	44,44,44,44	0
57	MG	1A	3197	1/1	0.72	0.32	55,55,55,55	0
57	MG	1m	3001	1/1	0.73	0.14	58,58,58,58	0
57	MG	2A	3329	1/1	0.73	0.14	75,75,75,75	0
57	MG	2A	3396	1/1	0.73	0.18	57,57,57,57	0
57	MG	1A	3315	1/1	0.73	0.15	56,56,56,56	0
57	MG	1A	3789	1/1	0.73	0.07	65,65,65,65	0
57	MG	1A	3673	1/1	0.73	0.21	38,38,38,38	0
57	MG	13	104	1/1	0.73	0.28	54,54,54,54	0
57	MG	1B	229	1/1	0.73	0.24	84,84,84,84	0
57	MG	1A	3266	1/1	0.73	0.22	70,70,70,70	0
57	MG	2A	3024	1/1	0.73	0.15	52,52,52,52	0
57	MG	1A	4022	1/1	0.73	0.06	68,68,68,68	0
57	MG	2A	3578	1/1	0.74	0.20	62,62,62,62	0
57	MG	2A	3599	1/1	0.74	0.18	62,62,62,62	0
57	MG	2A	3832	1/1	0.74	0.15	57,57,57,57	0
57	MG	1A	3431	1/1	0.74	0.25	56,56,56,56	0
57	MG	1A	3319	1/1	0.74	0.15	54,54,54,54	0
57	MG	2A	3196	1/1	0.74	0.14	54,54,54,54	0
57	MG	2F	302	1/1	0.74	0.12	64,64,64,64	0
57	MG	2A	3332	1/1	0.74	0.12	74,74,74,74	0
57	MG	2a	1714	1/1	0.74	0.29	77,77,77,77	0
57	MG	1a	1628	1/1	0.74	0.18	61,61,61,61	0
57	MG	1A	3299	1/1	0.74	0.39	51,51,51,51	0
57	MG	2A	3291	1/1	0.74	0.11	81,81,81,81	0
57	MG	1x	103	1/1	0.74	0.20	76,76,76,76	0
57	MG	2A	3764	1/1	0.74	0.12	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3561	1/1	0.74	0.12	40,40,40,40	0
57	MG	2A	3211	1/1	0.74	0.19	70,70,70,70	0
57	MG	2a	1658	1/1	0.75	0.18	63,63,63,63	0
57	MG	2A	3739	1/1	0.75	0.30	75,75,75,75	0
57	MG	2A	3194	1/1	0.75	0.12	64,64,64,64	0
57	MG	2A	3331	1/1	0.75	0.10	75,75,75,75	0
57	MG	1A	3338	1/1	0.75	0.21	42,42,42,42	0
57	MG	2A	3789	1/1	0.75	0.34	90,90,90,90	0
57	MG	1a	1642	1/1	0.75	0.19	71,71,71,71	0
57	MG	2a	1717	1/1	0.75	0.15	66,66,66,66	0
57	MG	2A	3629	1/1	0.75	0.22	52,52,52,52	0
57	MG	2a	1615	1/1	0.75	0.22	73,73,73,73	0
57	MG	2a	1778	1/1	0.75	0.17	80,80,80,80	0
57	MG	2a	1806	1/1	0.75	0.47	79,79,79,79	0
57	MG	1A	4069	1/1	0.75	0.22	51,51,51,51	0
57	MG	1A	3702	1/1	0.75	0.18	40,40,40,40	0
57	MG	1a	1674	1/1	0.75	0.17	70,70,70,70	0
57	MG	1A	3999	1/1	0.75	0.13	44,44,44,44	0
57	MG	1a	1630	1/1	0.75	0.24	68,68,68,68	0
57	MG	1B	215	1/1	0.76	0.13	63,63,63,63	0
57	MG	2A	3791	1/1	0.76	0.31	66,66,66,66	0
57	MG	1n	101	1/1	0.76	0.25	67,67,67,67	0
57	MG	2A	3264	1/1	0.76	0.19	62,62,62,62	0
57	MG	2A	3812	1/1	0.76	0.23	48,48,48,48	0
57	MG	1A	3535	1/1	0.76	0.24	57,57,57,57	0
57	MG	1A	3898	1/1	0.76	0.24	59,59,59,59	0
57	MG	2a	1700	1/1	0.76	0.13	62,62,62,62	0
57	MG	1A	3499	1/1	0.76	0.38	41,41,41,41	0
57	MG	1A	3624	1/1	0.76	0.20	24,24,24,24	0
57	MG	2A	3654	1/1	0.76	0.24	67,67,67,67	0
57	MG	2a	1716	1/1	0.76	0.24	77,77,77,77	0
57	MG	1a	1665	1/1	0.76	0.37	71,71,71,71	0
57	MG	2A	3665	1/1	0.76	0.18	52,52,52,52	0
57	MG	2a	1743	1/1	0.76	0.29	84,84,84,84	0
57	MG	2A	3310	1/1	0.76	0.42	64,64,64,64	0
57	MG	1A	3460	1/1	0.76	0.21	73,73,73,73	0
57	MG	2A	3387	1/1	0.76	0.14	69,69,69,69	0
57	MG	1A	3002	1/1	0.76	0.17	46,46,46,46	0
57	MG	2j	202	1/1	0.76	0.17	85,85,85,85	0
57	MG	1A	3688	1/1	0.76	0.11	38,38,38,38	0
57	MG	1A	3700	1/1	0.76	0.16	54,54,54,54	0
57	MG	2A	3438	1/1	0.76	0.13	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	4009	1/1	0.76	0.16	60,60,60,60	0
57	MG	2A	3793	1/1	0.77	0.10	56,56,56,56	0
57	MG	2A	3051	1/1	0.77	0.11	54,54,54,54	0
57	MG	1A	3697	1/1	0.77	0.20	55,55,55,55	0
57	MG	2A	3084	1/1	0.77	0.17	52,52,52,52	0
57	MG	1A	3444	1/1	0.77	0.33	61,61,61,61	0
57	MG	1A	3366	1/1	0.77	0.30	76,76,76,76	0
57	MG	2A	3342	1/1	0.77	0.14	62,62,62,62	0
57	MG	2A	3267	1/1	0.77	0.24	59,59,59,59	0
57	MG	1A	3632	1/1	0.77	0.11	48,48,48,48	0
57	MG	2A	3159	1/1	0.77	0.20	58,58,58,58	0
57	MG	2A	3676	1/1	0.77	0.13	61,61,61,61	0
57	MG	2A	3165	1/1	0.77	0.15	68,68,68,68	0
57	MG	26	101	1/1	0.77	0.16	64,64,64,64	0
57	MG	2A	3287	1/1	0.77	0.16	67,67,67,67	0
57	MG	1a	1664	1/1	0.77	0.31	55,55,55,55	0
57	MG	1A	3143	1/1	0.77	0.20	58,58,58,58	0
57	MG	2a	1812	1/1	0.77	0.10	76,76,76,76	0
57	MG	1E	309	1/1	0.77	0.14	68,68,68,68	0
57	MG	1A	3523	1/1	0.77	0.29	49,49,49,49	0
57	MG	1A	3415	1/1	0.77	0.36	42,42,42,42	0
57	MG	2w	103	1/1	0.77	0.15	79,79,79,79	0
57	MG	2A	3325	1/1	0.77	0.35	80,80,80,80	0
57	MG	1B	225	1/1	0.77	0.21	63,63,63,63	0
57	MG	1A	4029	1/1	0.77	0.08	58,58,58,58	0
57	MG	2a	1638	1/1	0.78	0.14	52,52,52,52	0
57	MG	2A	3756	1/1	0.78	0.12	69,69,69,69	0
57	MG	1a	1713	1/1	0.78	0.32	58,58,58,58	0
57	MG	1a	1651	1/1	0.78	0.40	67,67,67,67	0
57	MG	1R	206	1/1	0.78	0.19	41,41,41,41	0
57	MG	1A	3343	1/1	0.78	0.28	60,60,60,60	0
57	MG	2a	1660	1/1	0.78	0.09	64,64,64,64	0
57	MG	1a	1740	1/1	0.78	0.15	66,66,66,66	0
57	MG	1A	3472	1/1	0.78	0.18	67,67,67,67	0
57	MG	2a	1669	1/1	0.78	0.13	66,66,66,66	0
57	MG	2A	3583	1/1	0.78	0.10	69,69,69,69	0
57	MG	1a	1607	1/1	0.78	0.14	74,74,74,74	0
57	MG	2a	1703	1/1	0.78	0.17	79,79,79,79	0
57	MG	2a	1704	1/1	0.78	0.22	71,71,71,71	0
57	MG	2A	3602	1/1	0.78	0.12	60,60,60,60	0
57	MG	1a	1670	1/1	0.78	0.17	49,49,49,49	0
57	MG	2A	3063	1/1	0.78	0.10	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3214	1/1	0.78	0.18	49,49,49,49	0
57	MG	1a	1675	1/1	0.78	0.18	65,65,65,65	0
57	MG	1A	3399	1/1	0.78	0.15	51,51,51,51	0
57	MG	2a	1729	1/1	0.78	0.17	87,87,87,87	0
57	MG	2A	3095	1/1	0.78	0.15	55,55,55,55	0
57	MG	2a	1756	1/1	0.78	0.12	82,82,82,82	0
57	MG	2Q	202	1/1	0.78	0.23	58,58,58,58	0
57	MG	2A	3666	1/1	0.78	0.61	68,68,68,68	0
57	MG	1a	1680	1/1	0.78	0.21	77,77,77,77	0
57	MG	1A	3713	1/1	0.78	0.13	48,48,48,48	0
57	MG	1A	3567	1/1	0.78	0.14	71,71,71,71	0
57	MG	2A	3176	1/1	0.78	0.21	64,64,64,64	0
57	MG	2a	1607	1/1	0.78	0.13	66,66,66,66	0
57	MG	1A	3895	1/1	0.78	0.14	61,61,61,61	0
57	MG	1a	1711	1/1	0.78	0.13	67,67,67,67	0
57	MG	2a	1624	1/1	0.78	0.16	66,66,66,66	0
57	MG	2A	3411	1/1	0.78	0.17	61,61,61,61	0
57	MG	2a	1637	1/1	0.79	0.16	83,83,83,83	0
57	MG	1A	3144	1/1	0.79	0.20	42,42,42,42	0
57	MG	1l	102	1/1	0.79	0.30	75,75,75,75	0
57	MG	1A	3457	1/1	0.79	0.28	54,54,54,54	0
57	MG	1A	3409	1/1	0.79	0.19	55,55,55,55	0
57	MG	2A	3283	1/1	0.79	0.16	68,68,68,68	0
57	MG	2A	3786	1/1	0.79	0.20	58,58,58,58	0
57	MG	2A	3106	1/1	0.79	0.10	76,76,76,76	0
57	MG	2A	3430	1/1	0.79	0.13	41,41,41,41	0
57	MG	2A	3118	1/1	0.79	0.45	60,60,60,60	0
57	MG	2A	3455	1/1	0.79	0.17	58,58,58,58	0
57	MG	1B	221	1/1	0.79	0.28	62,62,62,62	0
57	MG	2A	3305	1/1	0.79	0.14	58,58,58,58	0
57	MG	1w	103	1/1	0.79	0.25	74,74,74,74	0
57	MG	2A	3166	1/1	0.79	0.10	67,67,67,67	0
57	MG	2A	3169	1/1	0.79	0.17	79,79,79,79	0
57	MG	2A	3836	1/1	0.79	0.09	50,50,50,50	0
57	MG	1A	3619	1/1	0.79	0.16	50,50,50,50	0
57	MG	2B	207	1/1	0.79	0.13	67,67,67,67	0
57	MG	2A	3186	1/1	0.79	0.47	72,72,72,72	0
57	MG	1A	3704	1/1	0.79	0.15	72,72,72,72	0
57	MG	1x	101	1/1	0.79	0.15	70,70,70,70	0
57	MG	2N	201	1/1	0.79	0.14	71,71,71,71	0
57	MG	1A	3507	1/1	0.79	0.17	56,56,56,56	0
57	MG	1A	3510	1/1	0.79	0.22	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3437	1/1	0.79	0.14	73,73,73,73	0
57	MG	2a	1803	1/1	0.79	0.11	61,61,61,61	0
57	MG	1A	3093	1/1	0.79	0.19	50,50,50,50	0
57	MG	1A	4053	1/1	0.79	0.23	31,31,31,31	0
57	MG	1a	1757	1/1	0.79	0.30	56,56,56,56	0
57	MG	1E	301	1/1	0.79	0.20	30,30,30,30	0
57	MG	1A	4059	1/1	0.79	0.30	63,63,63,63	0
57	MG	2A	3725	1/1	0.79	0.10	65,65,65,65	0
57	MG	2a	1620	1/1	0.79	0.13	74,74,74,74	0
57	MG	1A	3995	1/1	0.79	0.19	28,28,28,28	0
59	ZN	14	102	1/1	0.79	0.07	114,114,114,114	0
57	MG	1A	3793	1/1	0.79	0.09	62,62,62,62	0
57	MG	1a	1645	1/1	0.80	0.11	75,75,75,75	0
57	MG	2A	3306	1/1	0.80	0.23	74,74,74,74	0
57	MG	1A	3478	1/1	0.80	0.29	56,56,56,56	0
57	MG	2A	3473	1/1	0.80	0.12	62,62,62,62	0
57	MG	1A	4036	1/1	0.80	0.27	61,61,61,61	0
57	MG	2A	3502	1/1	0.80	0.09	59,59,59,59	0
57	MG	2A	3542	1/1	0.80	0.11	53,53,53,53	0
57	MG	1A	3417	1/1	0.80	0.20	66,66,66,66	0
57	MG	1A	3490	1/1	0.80	0.24	52,52,52,52	0
57	MG	1A	3967	1/1	0.80	0.12	52,52,52,52	0
57	MG	1a	1787	1/1	0.80	0.15	77,77,77,77	0
57	MG	1a	1789	1/1	0.80	0.16	70,70,70,70	0
57	MG	1A	3971	1/1	0.80	0.11	38,38,38,38	0
57	MG	1A	3786	1/1	0.80	0.20	34,34,34,34	0
57	MG	1A	3684	1/1	0.80	0.21	27,27,27,27	0
57	MG	2F	303	1/1	0.80	0.28	50,50,50,50	0
57	MG	2A	3232	1/1	0.80	0.53	57,57,57,57	0
57	MG	2A	3240	1/1	0.80	0.33	69,69,69,69	0
57	MG	1A	3293	1/1	0.80	0.20	55,55,55,55	0
57	MG	1A	3611	1/1	0.80	0.16	50,50,50,50	0
57	MG	2A	3351	1/1	0.80	0.19	76,76,76,76	0
57	MG	1A	3336	1/1	0.80	0.19	67,67,67,67	0
57	MG	2A	3678	1/1	0.80	0.50	68,68,68,68	0
57	MG	1A	3818	1/1	0.80	0.14	53,53,53,53	0
57	MG	2A	3150	1/1	0.80	0.16	66,66,66,66	0
57	MG	1a	1695	1/1	0.80	0.13	70,70,70,70	0
57	MG	2A	3282	1/1	0.80	0.10	65,65,65,65	0
57	MG	1A	3826	1/1	0.80	0.20	55,55,55,55	0
57	MG	2A	3390	1/1	0.80	0.12	76,76,76,76	0
57	MG	1A	3068	1/1	0.80	0.17	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2a	1627	1/1	0.80	0.23	68,68,68,68	0
57	MG	2x	104	1/1	0.80	0.15	64,64,64,64	0
57	MG	2A	3398	1/1	0.80	0.15	64,64,64,64	0
57	MG	1A	3870	1/1	0.80	0.12	62,62,62,62	0
57	MG	1A	3024	1/1	0.80	0.23	60,60,60,60	0
57	MG	10	107	1/1	0.81	0.17	56,56,56,56	0
57	MG	2D	303	1/1	0.81	0.17	68,68,68,68	0
57	MG	2A	3414	1/1	0.81	0.30	64,64,64,64	0
57	MG	2A	3245	1/1	0.81	0.18	63,63,63,63	0
57	MG	1A	3761	1/1	0.81	0.16	33,33,33,33	0
57	MG	2A	3436	1/1	0.81	0.20	65,65,65,65	0
57	MG	2A	3258	1/1	0.81	0.18	56,56,56,56	0
57	MG	2R	202	1/1	0.81	0.13	54,54,54,54	0
57	MG	1A	3943	1/1	0.81	0.15	45,45,45,45	0
57	MG	1A	3961	1/1	0.81	0.15	62,62,62,62	0
57	MG	2A	3476	1/1	0.81	0.26	70,70,70,70	0
57	MG	2A	3057	1/1	0.81	0.14	55,55,55,55	0
57	MG	1a	1626	1/1	0.81	0.19	53,53,53,53	0
57	MG	2A	3072	1/1	0.81	0.11	51,51,51,51	0
57	MG	1A	3629	1/1	0.81	0.17	46,46,46,46	0
57	MG	1A	3968	1/1	0.81	0.23	53,53,53,53	0
57	MG	1A	3446	1/1	0.81	0.17	54,54,54,54	0
57	MG	1A	3644	1/1	0.81	0.12	58,58,58,58	0
57	MG	1a	1778	1/1	0.81	0.07	68,68,68,68	0
57	MG	1A	3534	1/1	0.81	0.21	52,52,52,52	0
57	MG	2A	3111	1/1	0.81	0.28	71,71,71,71	0
57	MG	1A	3402	1/1	0.81	0.50	55,55,55,55	0
57	MG	2A	3131	1/1	0.81	0.13	44,44,44,44	0
57	MG	2A	3649	1/1	0.81	0.13	73,73,73,73	0
57	MG	1A	3550	1/1	0.81	0.18	59,59,59,59	0
57	MG	1a	1660	1/1	0.81	0.16	73,73,73,73	0
57	MG	1a	1661	1/1	0.81	0.10	65,65,65,65	0
57	MG	1A	3407	1/1	0.81	0.41	43,43,43,43	0
57	MG	1A	3585	1/1	0.81	0.28	56,56,56,56	0
57	MG	1A	3246	1/1	0.81	0.27	60,60,60,60	0
57	MG	1A	4017	1/1	0.81	0.12	44,44,44,44	0
57	MG	1A	3854	1/1	0.81	0.18	67,67,67,67	0
57	MG	2a	1682	1/1	0.81	0.10	71,71,71,71	0
57	MG	2A	3713	1/1	0.81	0.13	51,51,51,51	0
57	MG	1A	3466	1/1	0.81	0.21	65,65,65,65	0
57	MG	2A	3341	1/1	0.81	0.87	64,64,64,64	0
57	MG	1A	3876	1/1	0.81	0.07	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3270	1/1	0.81	0.31	47,47,47,47	0
57	MG	1A	3623	1/1	0.81	0.21	51,51,51,51	0
57	MG	2A	3197	1/1	0.81	0.22	66,66,66,66	0
57	MG	2A	3757	1/1	0.81	0.33	63,63,63,63	0
57	MG	2a	1718	1/1	0.81	0.10	61,61,61,61	0
57	MG	2A	3763	1/1	0.81	0.61	50,50,50,50	0
57	MG	2A	3353	1/1	0.81	0.15	68,68,68,68	0
57	MG	2A	3357	1/1	0.81	0.72	54,54,54,54	0
57	MG	1O	201	1/1	0.81	0.49	50,50,50,50	0
57	MG	1A	3208	1/1	0.81	0.20	32,32,32,32	0
57	MG	2A	3371	1/1	0.81	0.23	71,71,71,71	0
57	MG	2a	1779	1/1	0.81	0.12	66,66,66,66	0
57	MG	2A	3373	1/1	0.81	0.19	70,70,70,70	0
57	MG	2a	1805	1/1	0.81	0.15	82,82,82,82	0
57	MG	1x	106	1/1	0.81	0.23	62,62,62,62	0
57	MG	1a	1694	1/1	0.81	0.13	59,59,59,59	0
57	MG	2A	3811	1/1	0.81	0.16	56,56,56,56	0
57	MG	2A	3383	1/1	0.81	0.14	57,57,57,57	0
57	MG	2A	3216	1/1	0.81	0.26	57,57,57,57	0
57	MG	1x	110	1/1	0.81	0.13	70,70,70,70	0
57	MG	2A	3228	1/1	0.81	0.55	65,65,65,65	0
57	MG	2x	103	1/1	0.81	0.12	74,74,74,74	0
57	MG	1A	4044	1/1	0.81	0.07	49,49,49,49	0
57	MG	2A	3235	1/1	0.81	0.16	63,63,63,63	0
57	MG	2B	206	1/1	0.81	0.11	60,60,60,60	0
59	ZN	2Y	202	1/1	0.81	0.14	94,94,94,94	0
57	MG	2A	3399	1/1	0.81	0.20	47,47,47,47	0
57	MG	1A	3936	1/1	0.82	0.09	64,64,64,64	0
57	MG	2A	3023	1/1	0.82	0.25	67,67,67,67	0
57	MG	1A	3520	1/1	0.82	0.37	31,31,31,31	0
57	MG	1A	3259	1/1	0.82	0.17	34,34,34,34	0
57	MG	2A	3748	1/1	0.82	0.17	43,43,43,43	0
57	MG	1A	4030	1/1	0.82	0.11	45,45,45,45	0
57	MG	1A	3339	1/1	0.82	0.24	58,58,58,58	0
57	MG	2A	3055	1/1	0.82	0.17	58,58,58,58	0
57	MG	2A	3456	1/1	0.82	0.17	68,68,68,68	0
57	MG	1A	3130	1/1	0.82	0.12	64,64,64,64	0
57	MG	2A	3214	1/1	0.82	0.13	59,59,59,59	0
57	MG	2a	1657	1/1	0.82	0.13	87,87,87,87	0
57	MG	2A	3487	1/1	0.82	0.21	61,61,61,61	0
57	MG	1a	1663	1/1	0.82	0.17	66,66,66,66	0
57	MG	1A	3334	1/1	0.82	0.26	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3529	1/1	0.82	0.15	46,46,46,46	0
57	MG	1A	3358	1/1	0.82	0.14	42,42,42,42	0
57	MG	2a	1671	1/1	0.82	0.18	62,62,62,62	0
57	MG	2A	3807	1/1	0.82	0.13	55,55,55,55	0
57	MG	1a	1804	1/1	0.82	0.10	56,56,56,56	0
57	MG	2a	1697	1/1	0.82	0.19	70,70,70,70	0
57	MG	2A	3566	1/1	0.82	0.10	48,48,48,48	0
57	MG	1A	4049	1/1	0.82	0.14	49,49,49,49	0
57	MG	2A	3349	1/1	0.82	0.18	70,70,70,70	0
57	MG	1A	3864	1/1	0.82	0.12	52,52,52,52	0
57	MG	1F	310	1/1	0.82	0.18	47,47,47,47	0
57	MG	2A	3838	1/1	0.82	0.19	59,59,59,59	0
57	MG	2A	3857	1/1	0.82	0.09	73,73,73,73	0
57	MG	1A	3571	1/1	0.82	0.20	51,51,51,51	0
57	MG	2B	204	1/1	0.82	0.22	70,70,70,70	0
57	MG	1A	4064	1/1	0.82	0.15	54,54,54,54	0
57	MG	2A	3262	1/1	0.82	0.19	65,65,65,65	0
57	MG	1A	3365	1/1	0.82	0.10	60,60,60,60	0
57	MG	1A	3774	1/1	0.82	0.22	52,52,52,52	0
57	MG	2A	3651	1/1	0.82	0.11	55,55,55,55	0
57	MG	2A	3134	1/1	0.82	0.13	62,62,62,62	0
57	MG	2A	3660	1/1	0.82	0.11	50,50,50,50	0
57	MG	1A	4080	1/1	0.82	0.12	52,52,52,52	0
57	MG	1A	4081	1/1	0.82	0.22	21,21,21,21	0
57	MG	2Q	203	1/1	0.82	0.22	72,72,72,72	0
57	MG	16	102	1/1	0.82	0.29	59,59,59,59	0
57	MG	2W	201	1/1	0.82	0.14	64,64,64,64	0
57	MG	2A	3673	1/1	0.82	0.10	72,72,72,72	0
57	MG	23	102	1/1	0.82	0.31	60,60,60,60	0
57	MG	1A	3598	1/1	0.82	0.41	39,39,39,39	0
57	MG	1a	1696	1/1	0.82	0.11	59,59,59,59	0
57	MG	1A	3603	1/1	0.82	0.27	44,44,44,44	0
57	MG	2a	1604	1/1	0.82	0.18	71,71,71,71	0
57	MG	1A	3269	1/1	0.82	0.15	60,60,60,60	0
57	MG	1B	220	1/1	0.82	0.18	36,36,36,36	0
57	MG	2a	1611	1/1	0.82	0.16	69,69,69,69	0
57	MG	1A	3934	1/1	0.82	0.12	56,56,56,56	0
57	MG	1A	3678	1/1	0.83	0.19	24,24,24,24	0
57	MG	1a	1678	1/1	0.83	0.32	66,66,66,66	0
57	MG	1A	3222	1/1	0.83	0.15	42,42,42,42	0
57	MG	1A	4065	1/1	0.83	0.18	40,40,40,40	0
57	MG	1T	201	1/1	0.83	0.30	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	10	105	1/1	0.83	0.31	62,62,62,62	0
57	MG	1A	3386	1/1	0.83	0.46	42,42,42,42	0
57	MG	2A	3210	1/1	0.83	0.11	60,60,60,60	0
57	MG	1A	3302	1/1	0.83	0.44	71,71,71,71	0
57	MG	2A	3677	1/1	0.83	0.13	58,58,58,58	0
57	MG	2A	3016	1/1	0.83	0.17	68,68,68,68	0
57	MG	1A	3244	1/1	0.83	0.23	48,48,48,48	0
57	MG	1A	3065	1/1	0.83	0.24	55,55,55,55	0
57	MG	1a	1712	1/1	0.83	0.20	61,61,61,61	0
57	MG	1a	1601	1/1	0.83	0.42	68,68,68,68	0
57	MG	2a	1628	1/1	0.83	0.17	78,78,78,78	0
57	MG	2A	3727	1/1	0.83	0.12	59,59,59,59	0
57	MG	1a	1605	1/1	0.83	0.10	68,68,68,68	0
57	MG	1A	4082	1/1	0.83	0.16	34,34,34,34	0
57	MG	2A	3244	1/1	0.83	0.40	69,69,69,69	0
57	MG	2A	3742	1/1	0.83	0.17	41,41,41,41	0
57	MG	1A	3329	1/1	0.83	0.25	55,55,55,55	0
57	MG	1A	3707	1/1	0.83	0.21	39,39,39,39	0
57	MG	2A	3066	1/1	0.83	0.22	68,68,68,68	0
57	MG	2A	3071	1/1	0.83	0.23	50,50,50,50	0
57	MG	1A	3364	1/1	0.83	0.21	57,57,57,57	0
57	MG	1A	3414	1/1	0.83	0.21	39,39,39,39	0
57	MG	1A	3463	1/1	0.83	0.18	51,51,51,51	0
57	MG	1A	3333	1/1	0.83	0.28	58,58,58,58	0
57	MG	2A	3271	1/1	0.83	0.14	58,58,58,58	0
57	MG	2A	3435	1/1	0.83	0.15	65,65,65,65	0
57	MG	2a	1692	1/1	0.83	0.29	61,61,61,61	0
57	MG	1A	3767	1/1	0.83	0.19	40,40,40,40	0
57	MG	2A	3799	1/1	0.83	0.21	49,49,49,49	0
57	MG	1A	3902	1/1	0.83	0.19	32,32,32,32	0
57	MG	2A	3441	1/1	0.83	0.34	52,52,52,52	0
57	MG	1a	1794	1/1	0.83	0.20	50,50,50,50	0
57	MG	1A	3247	1/1	0.83	0.18	60,60,60,60	0
57	MG	2a	1713	1/1	0.83	0.10	79,79,79,79	0
57	MG	2A	3288	1/1	0.83	0.23	65,65,65,65	0
57	MG	1A	3776	1/1	0.83	0.23	15,15,15,15	0
57	MG	2A	3123	1/1	0.83	0.18	59,59,59,59	0
57	MG	1A	4040	1/1	0.83	0.14	44,44,44,44	0
57	MG	1a	1811	1/1	0.83	0.18	70,70,70,70	0
57	MG	2A	3505	1/1	0.83	0.11	72,72,72,72	0
57	MG	2A	3846	1/1	0.83	0.09	55,55,55,55	0
57	MG	1A	3782	1/1	0.83	0.20	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3315	1/1	0.83	0.14	53,53,53,53	0
57	MG	2A	3557	1/1	0.83	0.14	31,31,31,31	0
57	MG	2A	3316	1/1	0.83	0.44	68,68,68,68	0
57	MG	1A	3784	1/1	0.83	0.30	30,30,30,30	0
57	MG	2B	215	1/1	0.83	0.20	73,73,73,73	0
57	MG	1l	202	1/1	0.83	0.10	78,78,78,78	0
57	MG	1E	306	1/1	0.83	0.21	52,52,52,52	0
57	MG	2E	302	1/1	0.83	0.15	65,65,65,65	0
57	MG	2E	307	1/1	0.83	0.12	55,55,55,55	0
57	MG	1A	3945	1/1	0.83	0.08	49,49,49,49	0
57	MG	2w	101	1/1	0.83	0.09	70,70,70,70	0
57	MG	1r	101	1/1	0.83	0.21	72,72,72,72	0
57	MG	1A	3152	1/1	0.83	0.28	39,39,39,39	0
57	MG	1A	3424	1/1	0.83	0.15	55,55,55,55	0
57	MG	2P	201	1/1	0.83	0.15	68,68,68,68	0
57	MG	2A	3611	1/1	0.83	0.18	42,42,42,42	0
57	MG	2A	3189	1/1	0.83	0.14	64,64,64,64	0
57	MG	1I	201	1/1	0.83	0.14	62,62,62,62	0
57	MG	2A	3640	1/1	0.83	0.37	57,57,57,57	0
57	MG	2a	1629	1/1	0.84	0.15	76,76,76,76	0
57	MG	2a	1634	1/1	0.84	0.19	64,64,64,64	0
57	MG	1A	3724	1/1	0.84	0.23	26,26,26,26	0
57	MG	2A	3595	1/1	0.84	0.11	34,34,34,34	0
57	MG	2A	3377	1/1	0.84	0.17	61,61,61,61	0
57	MG	2A	3073	1/1	0.84	0.10	69,69,69,69	0
57	MG	2a	1646	1/1	0.84	0.10	73,73,73,73	0
57	MG	2A	3081	1/1	0.84	0.09	58,58,58,58	0
57	MG	1A	3899	1/1	0.84	0.21	30,30,30,30	0
57	MG	2A	3833	1/1	0.84	0.12	61,61,61,61	0
57	MG	2A	3613	1/1	0.84	0.27	56,56,56,56	0
57	MG	1A	3219	1/1	0.84	0.12	44,44,44,44	0
57	MG	1a	1618	1/1	0.84	0.12	43,43,43,43	0
57	MG	1A	3737	1/1	0.84	0.29	54,54,54,54	0
57	MG	2A	3847	1/1	0.84	0.11	51,51,51,51	0
57	MG	1A	3305	1/1	0.84	0.23	49,49,49,49	0
57	MG	2A	3101	1/1	0.84	0.13	72,72,72,72	0
57	MG	2A	3862	1/1	0.84	0.17	73,73,73,73	0
57	MG	2A	3409	1/1	0.84	0.18	39,39,39,39	0
57	MG	2a	1693	1/1	0.84	0.15	62,62,62,62	0
57	MG	1A	3416	1/1	0.84	0.19	69,69,69,69	0
57	MG	2A	3219	1/1	0.84	0.21	62,62,62,62	0
57	MG	2B	211	1/1	0.84	0.21	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3416	1/1	0.84	0.34	64,64,64,64	0
57	MG	1a	1681	1/1	0.84	0.21	63,63,63,63	0
57	MG	2A	3005	1/1	0.84	0.17	62,62,62,62	0
57	MG	2A	3120	1/1	0.84	0.22	57,57,57,57	0
57	MG	1B	209	1/1	0.84	0.12	41,41,41,41	0
57	MG	2A	3014	1/1	0.84	0.25	44,44,44,44	0
57	MG	1A	3942	1/1	0.84	0.14	27,27,27,27	0
57	MG	2A	3446	1/1	0.84	0.11	65,65,65,65	0
57	MG	2A	3140	1/1	0.84	0.10	73,73,73,73	0
57	MG	2A	3717	1/1	0.84	0.14	51,51,51,51	0
57	MG	1a	1636	1/1	0.84	0.24	72,72,72,72	0
57	MG	2A	3336	1/1	0.84	0.29	67,67,67,67	0
57	MG	2a	1761	1/1	0.84	0.16	67,67,67,67	0
57	MG	1A	3874	1/1	0.84	0.27	34,34,34,34	0
57	MG	1A	3058	1/1	0.84	0.20	42,42,42,42	0
57	MG	2A	3050	1/1	0.84	0.17	61,61,61,61	0
57	MG	2a	1796	1/1	0.84	0.13	72,72,72,72	0
57	MG	2A	3494	1/1	0.84	0.11	72,72,72,72	0
57	MG	25	101	1/1	0.84	0.12	56,56,56,56	0
57	MG	1A	3949	1/1	0.84	0.07	56,56,56,56	0
57	MG	2A	3504	1/1	0.84	0.10	64,64,64,64	0
57	MG	1A	4019	1/1	0.84	0.10	48,48,48,48	0
57	MG	2A	3515	1/1	0.84	0.10	58,58,58,58	0
57	MG	1A	3256	1/1	0.84	0.21	61,61,61,61	0
57	MG	2A	3270	1/1	0.84	0.32	63,63,63,63	0
57	MG	2A	3549	1/1	0.84	0.07	47,47,47,47	0
57	MG	2A	3783	1/1	0.84	0.11	53,53,53,53	0
57	MG	1A	3556	1/1	0.84	0.34	68,68,68,68	0
57	MG	1A	4068	1/1	0.84	0.10	37,37,37,37	0
57	MG	1A	4024	1/1	0.84	0.11	67,67,67,67	0
57	MG	2A	3568	1/1	0.84	0.18	45,45,45,45	0
57	MG	18	104	1/1	0.84	0.28	49,49,49,49	0
57	MG	2A	3284	1/1	0.84	0.21	61,61,61,61	0
57	MG	1A	3539	1/1	0.85	0.18	63,63,63,63	0
57	MG	1A	3656	1/1	0.85	0.21	52,52,52,52	0
57	MG	1e	202	1/1	0.85	0.26	52,52,52,52	0
57	MG	2A	3376	1/1	0.85	0.18	61,61,61,61	0
57	MG	1A	3665	1/1	0.85	0.16	26,26,26,26	0
57	MG	2A	3263	1/1	0.85	0.21	61,61,61,61	0
57	MG	2A	3381	1/1	0.85	0.17	65,65,65,65	0
57	MG	1A	3489	1/1	0.85	0.24	54,54,54,54	0
57	MG	1A	3551	1/1	0.85	0.27	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3552	1/1	0.85	0.26	59,59,59,59	0
57	MG	1A	3554	1/1	0.85	0.20	57,57,57,57	0
57	MG	1A	3958	1/1	0.85	0.18	31,31,31,31	0
57	MG	2A	3683	1/1	0.85	0.16	51,51,51,51	0
57	MG	2A	3695	1/1	0.85	0.07	63,63,63,63	0
57	MG	1A	3391	1/1	0.85	0.22	43,43,43,43	0
57	MG	1A	3558	1/1	0.85	0.11	65,65,65,65	0
57	MG	2A	3407	1/1	0.85	0.23	59,59,59,59	0
57	MG	1A	3123	1/1	0.85	0.18	40,40,40,40	0
57	MG	2A	3147	1/1	0.85	0.14	63,63,63,63	0
57	MG	1A	3394	1/1	0.85	0.35	60,60,60,60	0
57	MG	1A	3847	1/1	0.85	0.24	65,65,65,65	0
57	MG	2a	1636	1/1	0.85	0.24	65,65,65,65	0
57	MG	1A	4070	1/1	0.85	0.12	34,34,34,34	0
57	MG	1A	3853	1/1	0.85	0.17	65,65,65,65	0
57	MG	2a	1641	1/1	0.85	0.19	67,67,67,67	0
57	MG	2A	3743	1/1	0.85	0.12	60,60,60,60	0
57	MG	2A	3295	1/1	0.85	0.11	59,59,59,59	0
57	MG	2a	1645	1/1	0.85	0.10	65,65,65,65	0
57	MG	1A	3994	1/1	0.85	0.18	22,22,22,22	0
57	MG	2a	1647	1/1	0.85	0.10	69,69,69,69	0
57	MG	2A	3299	1/1	0.85	0.28	67,67,67,67	0
57	MG	2A	3172	1/1	0.85	0.47	63,63,63,63	0
57	MG	1A	3239	1/1	0.85	0.15	43,43,43,43	0
57	MG	2A	3308	1/1	0.85	0.24	68,68,68,68	0
57	MG	2A	3178	1/1	0.85	0.17	51,51,51,51	0
57	MG	2A	3462	1/1	0.85	0.30	65,65,65,65	0
57	MG	2A	3785	1/1	0.85	0.16	56,56,56,56	0
57	MG	2a	1666	1/1	0.85	0.13	62,62,62,62	0
57	MG	2A	3311	1/1	0.85	0.21	51,51,51,51	0
57	MG	1A	3508	1/1	0.85	0.20	50,50,50,50	0
57	MG	2A	3478	1/1	0.85	0.10	64,64,64,64	0
57	MG	17	105	1/1	0.85	0.21	51,51,51,51	0
57	MG	1A	4087	1/1	0.85	0.24	64,64,64,64	0
57	MG	2A	3489	1/1	0.85	0.19	63,63,63,63	0
57	MG	1A	3439	1/1	0.85	0.20	47,47,47,47	0
57	MG	2A	3324	1/1	0.85	0.15	62,62,62,62	0
57	MG	1A	4093	1/1	0.85	0.20	64,64,64,64	0
57	MG	1A	3467	1/1	0.85	0.33	44,44,44,44	0
57	MG	2A	3820	1/1	0.85	0.09	48,48,48,48	0
57	MG	1a	1612	1/1	0.85	0.15	65,65,65,65	0
57	MG	2A	3518	1/1	0.85	0.16	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3520	1/1	0.85	0.12	36,36,36,36	0
57	MG	2A	3524	1/1	0.85	0.15	71,71,71,71	0
57	MG	2A	3041	1/1	0.85	0.12	56,56,56,56	0
57	MG	1a	1615	1/1	0.85	0.18	67,67,67,67	0
57	MG	2A	3841	1/1	0.85	0.09	38,38,38,38	0
57	MG	1A	3440	1/1	0.85	0.13	44,44,44,44	0
57	MG	2A	3556	1/1	0.85	0.12	59,59,59,59	0
57	MG	2A	3053	1/1	0.85	0.18	71,71,71,71	0
57	MG	1B	210	1/1	0.85	0.11	52,52,52,52	0
57	MG	1A	3216	1/1	0.85	0.15	58,58,58,58	0
57	MG	1A	3883	1/1	0.85	0.14	36,36,36,36	0
57	MG	2B	205	1/1	0.85	0.12	70,70,70,70	0
57	MG	2a	1788	1/1	0.85	0.08	69,69,69,69	0
57	MG	2a	1791	1/1	0.85	0.12	64,64,64,64	0
57	MG	2a	1794	1/1	0.85	0.14	61,61,61,61	0
57	MG	1A	3526	1/1	0.85	0.42	47,47,47,47	0
57	MG	1B	223	1/1	0.85	0.23	55,55,55,55	0
57	MG	2B	209	1/1	0.85	0.20	75,75,75,75	0
57	MG	2A	3345	1/1	0.85	0.13	68,68,68,68	0
57	MG	2a	1811	1/1	0.85	0.16	64,64,64,64	0
57	MG	2A	3590	1/1	0.85	0.10	68,68,68,68	0
57	MG	1A	3530	1/1	0.85	0.11	73,73,73,73	0
57	MG	2a	1826	1/1	0.85	0.19	60,60,60,60	0
57	MG	2j	201	1/1	0.85	0.09	73,73,73,73	0
57	MG	2A	3598	1/1	0.85	0.17	58,58,58,58	0
57	MG	1A	3095	1/1	0.85	0.23	39,39,39,39	0
57	MG	2E	303	1/1	0.85	0.12	62,62,62,62	0
57	MG	1a	1643	1/1	0.85	0.18	63,63,63,63	0
57	MG	1A	3485	1/1	0.85	0.17	43,43,43,43	0
57	MG	2A	3354	1/1	0.85	0.26	64,64,64,64	0
57	MG	2A	3355	1/1	0.85	0.29	66,66,66,66	0
57	MG	2A	3239	1/1	0.85	0.19	51,51,51,51	0
57	MG	1a	1647	1/1	0.85	0.12	60,60,60,60	0
57	MG	1A	3907	1/1	0.85	0.25	45,45,45,45	0
57	MG	2A	3645	1/1	0.85	0.44	63,63,63,63	0
57	MG	1A	3089	1/1	0.86	0.26	34,34,34,34	0
57	MG	1A	3587	1/1	0.86	0.16	41,41,41,41	0
57	MG	2A	3285	1/1	0.86	0.15	57,57,57,57	0
57	MG	2A	3128	1/1	0.86	0.17	47,47,47,47	0
57	MG	2A	3419	1/1	0.86	0.26	57,57,57,57	0
57	MG	2A	3420	1/1	0.86	0.14	61,61,61,61	0
57	MG	2A	3710	1/1	0.86	0.20	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1a	1637	1/1	0.86	0.21	78,78,78,78	0
57	MG	2a	1618	1/1	0.86	0.15	70,70,70,70	0
57	MG	1A	4038	1/1	0.86	0.07	38,38,38,38	0
57	MG	2A	3433	1/1	0.86	0.14	51,51,51,51	0
57	MG	1A	3595	1/1	0.86	0.18	57,57,57,57	0
57	MG	2A	3296	1/1	0.86	0.30	68,68,68,68	0
57	MG	1A	3131	1/1	0.86	0.25	40,40,40,40	0
57	MG	2A	3738	1/1	0.86	0.11	60,60,60,60	0
57	MG	2a	1630	1/1	0.86	0.14	54,54,54,54	0
57	MG	1A	3258	1/1	0.86	0.14	22,22,22,22	0
57	MG	2A	3302	1/1	0.86	0.58	51,51,51,51	0
57	MG	2A	3448	1/1	0.86	0.53	49,49,49,49	0
57	MG	1D	309	1/1	0.86	0.18	47,47,47,47	0
57	MG	1A	3606	1/1	0.86	0.15	66,66,66,66	0
57	MG	2A	3752	1/1	0.86	0.12	62,62,62,62	0
57	MG	2a	1643	1/1	0.86	0.22	74,74,74,74	0
57	MG	1A	3845	1/1	0.86	0.15	46,46,46,46	0
57	MG	1A	3314	1/1	0.86	0.15	55,55,55,55	0
57	MG	1A	4054	1/1	0.86	0.12	62,62,62,62	0
57	MG	2A	3174	1/1	0.86	0.11	52,52,52,52	0
57	MG	1A	3966	1/1	0.86	0.21	47,47,47,47	0
57	MG	1A	3425	1/1	0.86	0.14	63,63,63,63	0
57	MG	2a	1656	1/1	0.86	0.11	76,76,76,76	0
57	MG	1F	315	1/1	0.86	0.29	55,55,55,55	0
57	MG	1A	3228	1/1	0.86	0.17	47,47,47,47	0
57	MG	2A	3495	1/1	0.86	0.18	64,64,64,64	0
57	MG	2A	3497	1/1	0.86	0.23	58,58,58,58	0
57	MG	1A	3622	1/1	0.86	0.23	31,31,31,31	0
57	MG	1O	205	1/1	0.86	0.20	67,67,67,67	0
57	MG	1a	1676	1/1	0.86	0.24	69,69,69,69	0
57	MG	1A	3869	1/1	0.86	0.15	66,66,66,66	0
57	MG	1A	3354	1/1	0.86	0.22	54,54,54,54	0
57	MG	2a	1680	1/1	0.86	0.16	73,73,73,73	0
57	MG	1A	3759	1/1	0.86	0.25	19,19,19,19	0
57	MG	1A	3484	1/1	0.86	0.14	43,43,43,43	0
57	MG	2A	3527	1/1	0.86	0.13	65,65,65,65	0
57	MG	1A	3996	1/1	0.86	0.17	31,31,31,31	0
57	MG	2A	3827	1/1	0.86	0.13	48,48,48,48	0
57	MG	2a	1701	1/1	0.86	0.08	75,75,75,75	0
57	MG	2A	3531	1/1	0.86	0.12	77,77,77,77	0
57	MG	1a	1689	1/1	0.86	0.30	66,66,66,66	0
57	MG	2A	3208	1/1	0.86	0.41	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3210	1/1	0.86	0.11	65,65,65,65	0
57	MG	1A	3404	1/1	0.86	0.37	37,37,37,37	0
57	MG	1A	3892	1/1	0.86	0.26	51,51,51,51	0
57	MG	2A	3842	1/1	0.86	0.13	56,56,56,56	0
57	MG	1A	3082	1/1	0.86	0.18	40,40,40,40	0
57	MG	18	101	1/1	0.86	0.52	52,52,52,52	0
57	MG	1A	4094	1/1	0.86	0.19	49,49,49,49	0
57	MG	1A	3441	1/1	0.86	0.20	52,52,52,52	0
57	MG	2A	3579	1/1	0.86	0.33	69,69,69,69	0
57	MG	2B	201	1/1	0.86	0.08	79,79,79,79	0
57	MG	1a	1604	1/1	0.86	0.10	55,55,55,55	0
57	MG	1A	3183	1/1	0.86	0.15	52,52,52,52	0
57	MG	2a	1768	1/1	0.86	0.12	82,82,82,82	0
57	MG	2a	1769	1/1	0.86	0.20	76,76,76,76	0
57	MG	2a	1771	1/1	0.86	0.08	75,75,75,75	0
57	MG	1a	1606	1/1	0.86	0.17	57,57,57,57	0
57	MG	1A	3410	1/1	0.86	0.18	48,48,48,48	0
57	MG	2a	1784	1/1	0.86	0.09	68,68,68,68	0
57	MG	2A	3070	1/1	0.86	0.12	51,51,51,51	0
57	MG	2A	3364	1/1	0.86	0.07	64,64,64,64	0
57	MG	1B	211	1/1	0.86	0.13	48,48,48,48	0
57	MG	1B	212	1/1	0.86	0.23	63,63,63,63	0
57	MG	2a	1801	1/1	0.86	0.13	61,61,61,61	0
57	MG	2A	3257	1/1	0.86	0.14	54,54,54,54	0
57	MG	2A	3614	1/1	0.86	0.09	65,65,65,65	0
57	MG	1a	1765	1/1	0.86	0.13	63,63,63,63	0
57	MG	2A	3626	1/1	0.86	0.12	49,49,49,49	0
57	MG	1A	3218	1/1	0.86	0.29	39,39,39,39	0
57	MG	2A	3633	1/1	0.86	0.11	44,44,44,44	0
57	MG	1a	1625	1/1	0.86	0.34	55,55,55,55	0
57	MG	2A	3380	1/1	0.86	0.26	51,51,51,51	0
57	MG	1a	1781	1/1	0.86	0.09	65,65,65,65	0
57	MG	2r	102	1/1	0.86	0.09	76,76,76,76	0
57	MG	1A	3914	1/1	0.86	0.21	45,45,45,45	0
57	MG	1A	3922	1/1	0.86	0.15	47,47,47,47	0
57	MG	2Q	204	1/1	0.86	0.29	56,56,56,56	0
57	MG	1B	222	1/1	0.86	0.24	48,48,48,48	0
57	MG	1A	3335	1/1	0.86	0.10	50,50,50,50	0
57	MG	1a	1802	1/1	0.86	0.11	52,52,52,52	0
57	MG	21	102	1/1	0.86	0.77	52,52,52,52	0
58	K	2A	3450	1/1	0.86	0.10	65,65,65,65	0
57	MG	2A	3272	1/1	0.86	0.13	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1a	1632	1/1	0.86	0.22	60,60,60,60	0
57	MG	1a	1805	1/1	0.86	0.11	54,54,54,54	0
57	MG	2a	1617	1/1	0.87	0.14	77,77,77,77	0
57	MG	2A	3075	1/1	0.87	0.25	40,40,40,40	0
57	MG	2A	3078	1/1	0.87	0.12	47,47,47,47	0
57	MG	2A	3491	1/1	0.87	0.18	71,71,71,71	0
57	MG	1A	3380	1/1	0.87	0.29	51,51,51,51	0
57	MG	2A	3745	1/1	0.87	0.14	34,34,34,34	0
57	MG	1A	3451	1/1	0.87	0.37	46,46,46,46	0
57	MG	2A	3085	1/1	0.87	0.31	58,58,58,58	0
57	MG	2A	3751	1/1	0.87	0.16	58,58,58,58	0
57	MG	2A	3500	1/1	0.87	0.11	74,74,74,74	0
57	MG	1l	201	1/1	0.87	0.15	59,59,59,59	0
57	MG	2A	3503	1/1	0.87	0.17	34,34,34,34	0
57	MG	1A	3577	1/1	0.87	0.26	42,42,42,42	0
57	MG	2a	1640	1/1	0.87	0.12	74,74,74,74	0
57	MG	2A	3348	1/1	0.87	0.14	65,65,65,65	0
57	MG	1A	3272	1/1	0.87	0.22	39,39,39,39	0
57	MG	1A	3429	1/1	0.87	0.13	44,44,44,44	0
57	MG	2A	3249	1/1	0.87	0.08	65,65,65,65	0
57	MG	2A	3352	1/1	0.87	0.11	67,67,67,67	0
57	MG	2A	3252	1/1	0.87	0.21	54,54,54,54	0
57	MG	1A	3493	1/1	0.87	0.17	56,56,56,56	0
57	MG	1A	3025	1/1	0.87	0.17	32,32,32,32	0
57	MG	2a	1652	1/1	0.87	0.39	62,62,62,62	0
57	MG	2A	3534	1/1	0.87	0.10	60,60,60,60	0
57	MG	2A	3539	1/1	0.87	0.25	49,49,49,49	0
57	MG	2A	3356	1/1	0.87	0.46	53,53,53,53	0
57	MG	1a	1617	1/1	0.87	0.11	62,62,62,62	0
57	MG	2A	3809	1/1	0.87	0.12	40,40,40,40	0
57	MG	1A	3546	1/1	0.87	0.32	61,61,61,61	0
57	MG	1A	3976	1/1	0.87	0.14	60,60,60,60	0
57	MG	1A	3295	1/1	0.87	0.12	39,39,39,39	0
57	MG	2A	3366	1/1	0.87	0.27	63,63,63,63	0
57	MG	2A	3369	1/1	0.87	0.24	49,49,49,49	0
57	MG	2A	3830	1/1	0.87	0.09	60,60,60,60	0
57	MG	2a	1679	1/1	0.87	0.10	70,70,70,70	0
57	MG	2A	3574	1/1	0.87	0.07	67,67,67,67	0
57	MG	2A	3126	1/1	0.87	0.13	43,43,43,43	0
57	MG	1A	3989	1/1	0.87	0.26	65,65,65,65	0
57	MG	1A	3887	1/1	0.87	0.15	26,26,26,26	0
57	MG	2a	1694	1/1	0.87	0.13	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3088	1/1	0.87	0.28	46,46,46,46	0
57	MG	2A	3137	1/1	0.87	0.18	49,49,49,49	0
57	MG	1a	1714	1/1	0.87	0.32	60,60,60,60	0
57	MG	2A	3142	1/1	0.87	0.12	52,52,52,52	0
57	MG	1A	3687	1/1	0.87	0.21	28,28,28,28	0
57	MG	1x	112	1/1	0.87	0.12	68,68,68,68	0
57	MG	2A	3154	1/1	0.87	0.20	66,66,66,66	0
57	MG	2a	1708	1/1	0.87	0.13	71,71,71,71	0
57	MG	2a	1711	1/1	0.87	0.13	67,67,67,67	0
57	MG	2A	3003	1/1	0.87	0.25	45,45,45,45	0
57	MG	1A	3615	1/1	0.87	0.12	60,60,60,60	0
57	MG	1A	3617	1/1	0.87	0.19	38,38,38,38	0
57	MG	2A	3620	1/1	0.87	0.08	51,51,51,51	0
57	MG	1A	3341	1/1	0.87	0.18	54,54,54,54	0
57	MG	1a	1743	1/1	0.87	0.19	56,56,56,56	0
57	MG	2A	3401	1/1	0.87	0.25	47,47,47,47	0
57	MG	2a	1737	1/1	0.87	0.10	70,70,70,70	0
57	MG	2a	1742	1/1	0.87	0.14	79,79,79,79	0
57	MG	1A	3182	1/1	0.87	0.24	38,38,38,38	0
57	MG	2B	214	1/1	0.87	0.14	68,68,68,68	0
57	MG	2A	3408	1/1	0.87	0.30	68,68,68,68	0
57	MG	2a	1762	1/1	0.87	0.11	70,70,70,70	0
57	MG	2A	3644	1/1	0.87	0.09	38,38,38,38	0
57	MG	2B	217	1/1	0.87	0.11	63,63,63,63	0
57	MG	1A	3620	1/1	0.87	0.19	47,47,47,47	0
57	MG	2E	301	1/1	0.87	0.30	57,57,57,57	0
57	MG	1A	3920	1/1	0.87	0.12	36,36,36,36	0
57	MG	2A	3300	1/1	0.87	0.17	60,60,60,60	0
57	MG	2A	3182	1/1	0.87	0.23	59,59,59,59	0
57	MG	2A	3655	1/1	0.87	0.12	68,68,68,68	0
57	MG	1A	3816	1/1	0.87	0.11	36,36,36,36	0
57	MG	2A	3042	1/1	0.87	0.20	59,59,59,59	0
57	MG	1A	3049	1/1	0.87	0.19	33,33,33,33	0
57	MG	2a	1799	1/1	0.87	0.20	56,56,56,56	0
57	MG	1A	3712	1/1	0.87	0.24	26,26,26,26	0
57	MG	2A	3052	1/1	0.87	0.17	54,54,54,54	0
57	MG	1A	3422	1/1	0.87	0.16	47,47,47,47	0
57	MG	1A	3940	1/1	0.87	0.10	50,50,50,50	0
57	MG	2a	1809	1/1	0.87	0.15	68,68,68,68	0
57	MG	13	103	1/1	0.87	0.13	46,46,46,46	0
57	MG	2A	3319	1/1	0.87	0.69	59,59,59,59	0
57	MG	20	101	1/1	0.87	0.20	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3321	1/1	0.87	0.31	57,57,57,57	0
57	MG	1A	3719	1/1	0.87	0.24	30,30,30,30	0
57	MG	2A	3696	1/1	0.87	0.06	58,58,58,58	0
57	MG	2q	201	1/1	0.87	0.13	65,65,65,65	0
57	MG	2A	3058	1/1	0.87	0.14	65,65,65,65	0
57	MG	2A	3707	1/1	0.87	0.56	64,64,64,64	0
57	MG	14	101	1/1	0.87	0.22	74,74,74,74	0
57	MG	2a	1601	1/1	0.87	0.14	61,61,61,61	0
57	MG	1A	4031	1/1	0.87	0.13	67,67,67,67	0
57	MG	2A	3471	1/1	0.87	0.17	54,54,54,54	0
57	MG	16	103	1/1	0.87	0.27	52,52,52,52	0
57	MG	1B	219	1/1	0.87	0.28	41,41,41,41	0
57	MG	1A	3722	1/1	0.87	0.21	52,52,52,52	0
57	MG	2a	1612	1/1	0.87	0.19	58,58,58,58	0
57	MG	1A	3849	1/1	0.87	0.13	59,59,59,59	0
57	MG	2A	3737	1/1	0.87	0.10	59,59,59,59	0
57	MG	1A	3073	1/1	0.88	0.23	51,51,51,51	0
57	MG	1A	3369	1/1	0.88	0.28	52,52,52,52	0
57	MG	10	108	1/1	0.88	0.22	60,60,60,60	0
57	MG	2A	3167	1/1	0.88	0.07	76,76,76,76	0
57	MG	2a	1621	1/1	0.88	0.14	75,75,75,75	0
57	MG	2A	3449	1/1	0.88	0.10	62,62,62,62	0
57	MG	2A	3732	1/1	0.88	0.10	70,70,70,70	0
57	MG	1x	108	1/1	0.88	0.16	35,35,35,35	0
57	MG	1A	3165	1/1	0.88	0.17	36,36,36,36	0
57	MG	2A	3312	1/1	0.88	0.23	60,60,60,60	0
57	MG	2A	3314	1/1	0.88	0.62	71,71,71,71	0
57	MG	1A	4079	1/1	0.88	0.10	49,49,49,49	0
57	MG	1A	3610	1/1	0.88	0.21	61,61,61,61	0
57	MG	1A	3170	1/1	0.88	0.15	30,30,30,30	0
57	MG	1a	1693	1/1	0.88	0.12	68,68,68,68	0
57	MG	2a	1639	1/1	0.88	0.24	62,62,62,62	0
57	MG	1A	3981	1/1	0.88	0.52	49,49,49,49	0
57	MG	1A	3863	1/1	0.88	0.13	68,68,68,68	0
57	MG	1A	3612	1/1	0.88	0.10	63,63,63,63	0
57	MG	1A	3075	1/1	0.88	0.19	24,24,24,24	0
57	MG	1a	1706	1/1	0.88	0.15	64,64,64,64	0
57	MG	2A	3039	1/1	0.88	0.17	72,72,72,72	0
57	MG	1A	3252	1/1	0.88	0.11	59,59,59,59	0
57	MG	1A	3471	1/1	0.88	0.20	31,31,31,31	0
57	MG	2A	3045	1/1	0.88	0.07	70,70,70,70	0
57	MG	2A	3047	1/1	0.88	0.16	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3203	1/1	0.88	0.10	64,64,64,64	0
57	MG	2A	3513	1/1	0.88	0.12	71,71,71,71	0
57	MG	1a	1603	1/1	0.88	0.12	57,57,57,57	0
57	MG	2A	3338	1/1	0.88	0.69	52,52,52,52	0
57	MG	2A	3796	1/1	0.88	0.12	52,52,52,52	0
57	MG	2A	3339	1/1	0.88	0.30	59,59,59,59	0
57	MG	1A	3029	1/1	0.88	0.19	29,29,29,29	0
57	MG	2A	3526	1/1	0.88	0.36	69,69,69,69	0
57	MG	1a	1718	1/1	0.88	0.13	54,54,54,54	0
57	MG	1A	3736	1/1	0.88	0.10	50,50,50,50	0
57	MG	1A	3187	1/1	0.88	0.14	36,36,36,36	0
57	MG	2A	3215	1/1	0.88	0.10	66,66,66,66	0
57	MG	1A	4008	1/1	0.88	0.05	65,65,65,65	0
57	MG	2a	1681	1/1	0.88	0.12	62,62,62,62	0
57	MG	2A	3823	1/1	0.88	0.18	36,36,36,36	0
57	MG	2a	1683	1/1	0.88	0.12	64,64,64,64	0
57	MG	2A	3218	1/1	0.88	0.66	41,41,41,41	0
57	MG	1a	1610	1/1	0.88	0.10	66,66,66,66	0
57	MG	2A	3553	1/1	0.88	0.15	34,34,34,34	0
57	MG	1A	3751	1/1	0.88	0.15	60,60,60,60	0
57	MG	2A	3225	1/1	0.88	0.33	42,42,42,42	0
57	MG	1a	1745	1/1	0.88	0.12	69,69,69,69	0
57	MG	2A	3229	1/1	0.88	0.51	67,67,67,67	0
57	MG	2A	3231	1/1	0.88	0.07	70,70,70,70	0
57	MG	1A	3752	1/1	0.88	0.11	45,45,45,45	0
57	MG	2A	3359	1/1	0.88	0.11	69,69,69,69	0
57	MG	2A	3843	1/1	0.88	0.12	37,37,37,37	0
57	MG	1A	3479	1/1	0.88	0.19	47,47,47,47	0
57	MG	1A	3433	1/1	0.88	0.14	41,41,41,41	0
57	MG	1A	3482	1/1	0.88	0.13	61,61,61,61	0
57	MG	1A	3628	1/1	0.88	0.14	32,32,32,32	0
57	MG	1A	3345	1/1	0.88	0.17	56,56,56,56	0
57	MG	2A	3597	1/1	0.88	0.13	55,55,55,55	0
57	MG	2A	3370	1/1	0.88	0.29	65,65,65,65	0
57	MG	2a	1722	1/1	0.88	0.25	69,69,69,69	0
57	MG	2a	1723	1/1	0.88	0.19	71,71,71,71	0
57	MG	2a	1726	1/1	0.88	0.21	63,63,63,63	0
57	MG	2a	1728	1/1	0.88	0.09	61,61,61,61	0
57	MG	1A	3044	1/1	0.88	0.20	39,39,39,39	0
57	MG	2A	3079	1/1	0.88	0.13	59,59,59,59	0
57	MG	2A	3604	1/1	0.88	0.17	57,57,57,57	0
57	MG	1A	3916	1/1	0.88	0.12	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2B	210	1/1	0.88	0.26	68,68,68,68	0
57	MG	2a	1757	1/1	0.88	0.12	61,61,61,61	0
57	MG	1A	3264	1/1	0.88	0.14	69,69,69,69	0
57	MG	2B	213	1/1	0.88	0.12	72,72,72,72	0
57	MG	1A	3557	1/1	0.88	0.24	57,57,57,57	0
57	MG	2a	1767	1/1	0.88	0.23	72,72,72,72	0
57	MG	1A	3265	1/1	0.88	0.14	41,41,41,41	0
57	MG	1A	3491	1/1	0.88	0.21	36,36,36,36	0
57	MG	1a	1640	1/1	0.88	0.09	56,56,56,56	0
57	MG	1A	3670	1/1	0.88	0.15	36,36,36,36	0
57	MG	2A	3627	1/1	0.88	0.18	53,53,53,53	0
57	MG	2A	3384	1/1	0.88	0.19	61,61,61,61	0
57	MG	2A	3385	1/1	0.88	0.13	67,67,67,67	0
57	MG	1A	3798	1/1	0.88	0.13	43,43,43,43	0
57	MG	1A	4045	1/1	0.88	0.15	58,58,58,58	0
57	MG	1A	3359	1/1	0.88	0.16	47,47,47,47	0
57	MG	2A	3395	1/1	0.88	0.10	70,70,70,70	0
57	MG	1A	3576	1/1	0.88	0.27	38,38,38,38	0
57	MG	1E	315	1/1	0.88	0.23	55,55,55,55	0
57	MG	2A	3274	1/1	0.88	0.46	47,47,47,47	0
57	MG	2A	3659	1/1	0.88	0.17	51,51,51,51	0
57	MG	1A	4052	1/1	0.88	0.24	33,33,33,33	0
57	MG	1A	3809	1/1	0.88	0.23	51,51,51,51	0
57	MG	2T	3501	1/1	0.88	0.20	66,66,66,66	0
57	MG	2A	3127	1/1	0.88	0.13	69,69,69,69	0
57	MG	2a	1821	1/1	0.88	0.15	62,62,62,62	0
57	MG	1A	3323	1/1	0.88	0.27	36,36,36,36	0
57	MG	2A	3130	1/1	0.88	0.13	48,48,48,48	0
57	MG	2A	3413	1/1	0.88	0.21	67,67,67,67	0
57	MG	1A	4056	1/1	0.88	0.12	42,42,42,42	0
57	MG	1A	3952	1/1	0.88	0.12	26,26,26,26	0
57	MG	1R	205	1/1	0.88	0.33	43,43,43,43	0
57	MG	1w	104	1/1	0.88	0.10	67,67,67,67	0
57	MG	2A	3694	1/1	0.88	0.38	69,69,69,69	0
57	MG	1A	3200	1/1	0.88	0.14	47,47,47,47	0
57	MG	2A	3297	1/1	0.88	0.14	45,45,45,45	0
57	MG	2A	3705	1/1	0.88	0.14	33,33,33,33	0
57	MG	1A	3448	1/1	0.88	0.11	37,37,37,37	0
57	MG	2a	1608	1/1	0.88	0.25	64,64,64,64	0
57	MG	1A	3204	1/1	0.88	0.15	43,43,43,43	0
57	MG	2A	3709	1/1	0.88	0.13	60,60,60,60	0
57	MG	1U	203	1/1	0.88	0.24	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1O	204	1/1	0.89	0.15	56,56,56,56	0
57	MG	1A	4061	1/1	0.89	0.16	63,63,63,63	0
57	MG	2A	3143	1/1	0.89	0.26	40,40,40,40	0
57	MG	2A	3145	1/1	0.89	0.15	55,55,55,55	0
57	MG	1A	3970	1/1	0.89	0.10	54,54,54,54	0
57	MG	1A	3387	1/1	0.89	0.15	54,54,54,54	0
57	MG	1S	202	1/1	0.89	0.15	55,55,55,55	0
57	MG	2a	1626	1/1	0.89	0.28	60,60,60,60	0
57	MG	1w	109	1/1	0.89	0.13	71,71,71,71	0
57	MG	1A	4066	1/1	0.89	0.17	53,53,53,53	0
57	MG	1A	3411	1/1	0.89	0.13	41,41,41,41	0
57	MG	1A	3555	1/1	0.89	0.28	57,57,57,57	0
57	MG	1U	204	1/1	0.89	0.18	26,26,26,26	0
57	MG	2a	1635	1/1	0.89	0.20	66,66,66,66	0
57	MG	1A	3681	1/1	0.89	0.13	52,52,52,52	0
57	MG	1A	3982	1/1	0.89	0.19	53,53,53,53	0
57	MG	2A	3485	1/1	0.89	0.27	73,73,73,73	0
57	MG	2A	3317	1/1	0.89	0.81	54,54,54,54	0
57	MG	1A	3880	1/1	0.89	0.23	66,66,66,66	0
57	MG	1x	111	1/1	0.89	0.10	57,57,57,57	0
57	MG	10	109	1/1	0.89	0.11	43,43,43,43	0
57	MG	11	101	1/1	0.89	0.08	43,43,43,43	0
57	MG	1a	1691	1/1	0.89	0.13	74,74,74,74	0
57	MG	1A	3985	1/1	0.89	0.16	48,48,48,48	0
57	MG	2A	3326	1/1	0.89	0.52	56,56,56,56	0
57	MG	1A	3297	1/1	0.89	0.17	60,60,60,60	0
57	MG	1A	3992	1/1	0.89	0.15	30,30,30,30	0
57	MG	2A	3784	1/1	0.89	0.10	73,73,73,73	0
57	MG	2a	1653	1/1	0.89	0.09	62,62,62,62	0
57	MG	1A	3522	1/1	0.89	0.23	37,37,37,37	0
57	MG	1A	3241	1/1	0.89	0.18	32,32,32,32	0
57	MG	2A	3030	1/1	0.89	0.08	38,38,38,38	0
57	MG	2A	3514	1/1	0.89	0.14	40,40,40,40	0
57	MG	2A	3031	1/1	0.89	0.14	56,56,56,56	0
57	MG	1a	1702	1/1	0.89	0.32	61,61,61,61	0
57	MG	2A	3202	1/1	0.89	0.42	53,53,53,53	0
57	MG	1A	4092	1/1	0.89	0.12	47,47,47,47	0
57	MG	2a	1667	1/1	0.89	0.14	64,64,64,64	0
57	MG	1A	3559	1/1	0.89	0.19	60,60,60,60	0
57	MG	1A	3261	1/1	0.89	0.14	49,49,49,49	0
57	MG	2A	3209	1/1	0.89	0.15	57,57,57,57	0
57	MG	1A	4097	1/1	0.89	0.09	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3209	1/1	0.89	0.15	48,48,48,48	0
57	MG	2A	3817	1/1	0.89	0.06	57,57,57,57	0
57	MG	2A	3212	1/1	0.89	0.08	66,66,66,66	0
57	MG	1a	1602	1/1	0.89	0.10	69,69,69,69	0
57	MG	1a	1717	1/1	0.89	0.14	53,53,53,53	0
57	MG	1A	3419	1/1	0.89	0.21	50,50,50,50	0
57	MG	1A	3468	1/1	0.89	0.17	59,59,59,59	0
57	MG	1A	3711	1/1	0.89	0.07	63,63,63,63	0
57	MG	1A	3376	1/1	0.89	0.34	40,40,40,40	0
57	MG	1A	3627	1/1	0.89	0.25	52,52,52,52	0
57	MG	1a	1742	1/1	0.89	0.19	64,64,64,64	0
57	MG	2A	3062	1/1	0.89	0.25	58,58,58,58	0
57	MG	2A	3230	1/1	0.89	0.31	62,62,62,62	0
57	MG	1A	3817	1/1	0.89	0.07	38,38,38,38	0
57	MG	1A	3541	1/1	0.89	0.19	42,42,42,42	0
57	MG	2A	3363	1/1	0.89	0.24	62,62,62,62	0
57	MG	2A	3585	1/1	0.89	0.13	61,61,61,61	0
57	MG	2A	3855	1/1	0.89	0.23	63,63,63,63	0
57	MG	1a	1755	1/1	0.89	0.11	56,56,56,56	0
57	MG	1A	3824	1/1	0.89	0.14	31,31,31,31	0
57	MG	2A	3367	1/1	0.89	0.09	52,52,52,52	0
57	MG	1A	3591	1/1	0.89	0.14	33,33,33,33	0
57	MG	1A	4027	1/1	0.89	0.23	52,52,52,52	0
57	MG	1a	1623	1/1	0.89	0.08	70,70,70,70	0
57	MG	1A	3935	1/1	0.89	0.16	38,38,38,38	0
57	MG	2A	3607	1/1	0.89	0.12	31,31,31,31	0
57	MG	2B	208	1/1	0.89	0.11	70,70,70,70	0
57	MG	1A	3592	1/1	0.89	0.12	37,37,37,37	0
57	MG	2A	3254	1/1	0.89	0.12	64,64,64,64	0
57	MG	2A	3080	1/1	0.89	0.16	52,52,52,52	0
57	MG	2a	1752	1/1	0.89	0.14	66,66,66,66	0
57	MG	1A	3834	1/1	0.89	0.16	59,59,59,59	0
57	MG	2A	3619	1/1	0.89	0.13	72,72,72,72	0
57	MG	1A	4033	1/1	0.89	0.22	69,69,69,69	0
57	MG	1A	3730	1/1	0.89	0.20	44,44,44,44	0
57	MG	2a	1763	1/1	0.89	0.14	69,69,69,69	0
57	MG	1A	3636	1/1	0.89	0.24	35,35,35,35	0
57	MG	1A	3181	1/1	0.89	0.19	56,56,56,56	0
57	MG	2A	3094	1/1	0.89	0.18	72,72,72,72	0
57	MG	1a	1635	1/1	0.89	0.09	56,56,56,56	0
57	MG	2A	3635	1/1	0.89	0.18	64,64,64,64	0
57	MG	2a	1772	1/1	0.89	0.14	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3946	1/1	0.89	0.11	42,42,42,42	0
57	MG	1A	3654	1/1	0.89	0.13	48,48,48,48	0
57	MG	2a	1782	1/1	0.89	0.14	50,50,50,50	0
57	MG	2a	1783	1/1	0.89	0.15	64,64,64,64	0
57	MG	2A	3392	1/1	0.89	0.16	53,53,53,53	0
57	MG	2F	304	1/1	0.89	0.22	60,60,60,60	0
57	MG	2F	306	1/1	0.89	0.45	51,51,51,51	0
57	MG	1A	3383	1/1	0.89	0.11	49,49,49,49	0
57	MG	1a	1814	1/1	0.89	0.28	76,76,76,76	0
57	MG	1a	1816	1/1	0.89	0.09	64,64,64,64	0
57	MG	2A	3275	1/1	0.89	0.41	66,66,66,66	0
57	MG	2A	3277	1/1	0.89	0.34	59,59,59,59	0
57	MG	2A	3278	1/1	0.89	0.27	67,67,67,67	0
57	MG	1a	1817	1/1	0.89	0.25	64,64,64,64	0
57	MG	1A	3859	1/1	0.89	0.08	63,63,63,63	0
57	MG	2V	203	1/1	0.89	0.22	67,67,67,67	0
57	MG	2A	3410	1/1	0.89	0.28	48,48,48,48	0
57	MG	2a	1814	1/1	0.89	0.17	78,78,78,78	0
57	MG	2a	1816	1/1	0.89	0.19	66,66,66,66	0
57	MG	2Z	301	1/1	0.89	0.10	74,74,74,74	0
57	MG	2A	3669	1/1	0.89	0.16	52,52,52,52	0
57	MG	2A	3124	1/1	0.89	0.15	70,70,70,70	0
57	MG	2d	301	1/1	0.89	0.31	62,62,62,62	0
57	MG	2A	3412	1/1	0.89	0.29	49,49,49,49	0
57	MG	1E	311	1/1	0.89	0.20	26,26,26,26	0
57	MG	2l	203	1/1	0.89	0.11	73,73,73,73	0
57	MG	1A	3860	1/1	0.89	0.07	52,52,52,52	0
57	MG	1A	3962	1/1	0.89	0.08	47,47,47,47	0
57	MG	28	102	1/1	0.89	0.16	48,48,48,48	0
57	MG	1A	3964	1/1	0.89	0.13	61,61,61,61	0
57	MG	2A	3689	1/1	0.89	0.08	62,62,62,62	0
57	MG	2A	3289	1/1	0.89	0.44	65,65,65,65	0
57	MG	1A	3861	1/1	0.89	0.14	56,56,56,56	0
57	MG	2A	3429	1/1	0.89	0.13	49,49,49,49	0
57	MG	2A	3700	1/1	0.89	0.12	71,71,71,71	0
57	MG	1A	3087	1/1	0.89	0.23	29,29,29,29	0
57	MG	1A	3604	1/1	0.89	0.32	64,64,64,64	0
57	MG	2A	3434	1/1	0.89	0.18	53,53,53,53	0
57	MG	2A	3708	1/1	0.89	0.20	66,66,66,66	0
57	MG	1A	3886	1/1	0.90	0.31	33,33,33,33	0
57	MG	1A	3427	1/1	0.90	0.19	55,55,55,55	0
57	MG	2A	3170	1/1	0.90	0.12	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3172	1/1	0.90	0.17	51,51,51,51	0
57	MG	2a	1619	1/1	0.90	0.11	78,78,78,78	0
57	MG	2A	3459	1/1	0.90	0.19	47,47,47,47	0
57	MG	2A	3461	1/1	0.90	0.30	69,69,69,69	0
57	MG	1A	3521	1/1	0.90	0.42	35,35,35,35	0
57	MG	2A	3718	1/1	0.90	0.11	60,60,60,60	0
57	MG	2A	3720	1/1	0.90	0.14	60,60,60,60	0
57	MG	2A	3465	1/1	0.90	0.12	55,55,55,55	0
57	MG	2A	3469	1/1	0.90	0.15	57,57,57,57	0
57	MG	2A	3729	1/1	0.90	0.10	69,69,69,69	0
57	MG	1B	202	1/1	0.90	0.30	54,54,54,54	0
57	MG	2A	3177	1/1	0.90	0.08	45,45,45,45	0
57	MG	1a	1707	1/1	0.90	0.13	63,63,63,63	0
57	MG	1a	1709	1/1	0.90	0.24	62,62,62,62	0
57	MG	2A	3481	1/1	0.90	0.12	50,50,50,50	0
57	MG	2A	3483	1/1	0.90	0.23	64,64,64,64	0
57	MG	2A	3018	1/1	0.90	0.16	58,58,58,58	0
57	MG	1A	3897	1/1	0.90	0.11	38,38,38,38	0
57	MG	1A	3363	1/1	0.90	0.20	39,39,39,39	0
57	MG	1A	3271	1/1	0.90	0.23	44,44,44,44	0
57	MG	2A	3747	1/1	0.90	0.32	43,43,43,43	0
57	MG	1A	3436	1/1	0.90	0.42	46,46,46,46	0
57	MG	2A	3032	1/1	0.90	0.12	44,44,44,44	0
57	MG	1A	3331	1/1	0.90	0.26	58,58,58,58	0
57	MG	1A	4013	1/1	0.90	0.19	37,37,37,37	0
57	MG	1A	3909	1/1	0.90	0.16	29,29,29,29	0
57	MG	1a	1723	1/1	0.90	0.25	61,61,61,61	0
57	MG	2A	3043	1/1	0.90	0.11	68,68,68,68	0
57	MG	2A	3766	1/1	0.90	0.07	73,73,73,73	0
57	MG	2A	3769	1/1	0.90	0.09	57,57,57,57	0
57	MG	1a	1725	1/1	0.90	0.15	49,49,49,49	0
57	MG	1A	3913	1/1	0.90	0.16	30,30,30,30	0
57	MG	2A	3207	1/1	0.90	0.19	70,70,70,70	0
57	MG	1a	1728	1/1	0.90	0.19	50,50,50,50	0
57	MG	1A	3250	1/1	0.90	0.22	58,58,58,58	0
57	MG	2A	3787	1/1	0.90	0.17	45,45,45,45	0
57	MG	1A	3207	1/1	0.90	0.12	60,60,60,60	0
57	MG	1A	3808	1/1	0.90	0.16	80,80,80,80	0
57	MG	1A	3483	1/1	0.90	0.15	53,53,53,53	0
57	MG	2A	3213	1/1	0.90	0.21	63,63,63,63	0
57	MG	1A	3227	1/1	0.90	0.15	41,41,41,41	0
57	MG	2A	3347	1/1	0.90	0.26	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3927	1/1	0.90	0.25	39,39,39,39	0
57	MG	1A	3542	1/1	0.90	0.28	53,53,53,53	0
57	MG	1a	1758	1/1	0.90	0.16	57,57,57,57	0
57	MG	2a	1688	1/1	0.90	0.25	65,65,65,65	0
57	MG	1a	1761	1/1	0.90	0.14	36,36,36,36	0
57	MG	1a	1763	1/1	0.90	0.08	65,65,65,65	0
57	MG	2A	3550	1/1	0.90	0.10	38,38,38,38	0
57	MG	2a	1695	1/1	0.90	0.13	80,80,80,80	0
57	MG	2A	3552	1/1	0.90	0.11	50,50,50,50	0
57	MG	2A	3068	1/1	0.90	0.14	38,38,38,38	0
57	MG	1A	3413	1/1	0.90	0.24	35,35,35,35	0
57	MG	1B	231	1/1	0.90	0.19	59,59,59,59	0
57	MG	1A	3486	1/1	0.90	0.44	52,52,52,52	0
57	MG	2A	3563	1/1	0.90	0.12	39,39,39,39	0
57	MG	1A	3487	1/1	0.90	0.18	38,38,38,38	0
57	MG	1a	1782	1/1	0.90	0.10	75,75,75,75	0
57	MG	2A	3233	1/1	0.90	0.59	57,57,57,57	0
57	MG	2A	3234	1/1	0.90	0.72	49,49,49,49	0
57	MG	2A	3840	1/1	0.90	0.19	60,60,60,60	0
57	MG	2A	3076	1/1	0.90	0.13	40,40,40,40	0
57	MG	2A	3236	1/1	0.90	0.38	61,61,61,61	0
57	MG	1A	4037	1/1	0.90	0.15	56,56,56,56	0
57	MG	1A	3488	1/1	0.90	0.14	59,59,59,59	0
57	MG	2A	3242	1/1	0.90	0.21	62,62,62,62	0
57	MG	1A	3019	1/1	0.90	0.21	50,50,50,50	0
57	MG	1A	4042	1/1	0.90	0.09	47,47,47,47	0
57	MG	2A	3858	1/1	0.90	0.16	64,64,64,64	0
57	MG	1A	3236	1/1	0.90	0.18	53,53,53,53	0
57	MG	2a	1733	1/1	0.90	0.35	65,65,65,65	0
57	MG	2A	3374	1/1	0.90	0.24	67,67,67,67	0
57	MG	2a	1739	1/1	0.90	0.25	75,75,75,75	0
57	MG	2a	1740	1/1	0.90	0.19	74,74,74,74	0
57	MG	2a	1741	1/1	0.90	0.14	70,70,70,70	0
57	MG	2A	3601	1/1	0.90	0.16	64,64,64,64	0
57	MG	2A	3250	1/1	0.90	0.30	50,50,50,50	0
57	MG	2a	1747	1/1	0.90	0.73	77,77,77,77	0
57	MG	2a	1748	1/1	0.90	0.13	68,68,68,68	0
57	MG	1A	3163	1/1	0.90	0.24	46,46,46,46	0
57	MG	2A	3253	1/1	0.90	0.26	58,58,58,58	0
57	MG	2A	3608	1/1	0.90	0.14	29,29,29,29	0
57	MG	2A	3378	1/1	0.90	0.28	75,75,75,75	0
57	MG	1E	314	1/1	0.90	0.46	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3728	1/1	0.90	0.18	55,55,55,55	0
57	MG	1A	3851	1/1	0.90	0.13	34,34,34,34	0
57	MG	1A	3492	1/1	0.90	0.12	44,44,44,44	0
57	MG	1A	3959	1/1	0.90	0.18	26,26,26,26	0
57	MG	1a	1657	1/1	0.90	0.19	43,43,43,43	0
57	MG	1A	3960	1/1	0.90	0.20	64,64,64,64	0
57	MG	2A	3108	1/1	0.90	0.17	55,55,55,55	0
57	MG	2a	1776	1/1	0.90	0.17	50,50,50,50	0
57	MG	2A	3109	1/1	0.90	0.17	66,66,66,66	0
57	MG	2A	3632	1/1	0.90	0.14	41,41,41,41	0
57	MG	1A	3133	1/1	0.90	0.20	37,37,37,37	0
57	MG	1A	3307	1/1	0.90	0.14	31,31,31,31	0
57	MG	2E	305	1/1	0.90	0.12	56,56,56,56	0
57	MG	2A	3638	1/1	0.90	0.14	43,43,43,43	0
57	MG	1f	201	1/1	0.90	0.22	53,53,53,53	0
57	MG	1P	203	1/1	0.90	0.23	28,28,28,28	0
57	MG	1P	205	1/1	0.90	0.08	35,35,35,35	0
57	MG	1A	3027	1/1	0.90	0.16	70,70,70,70	0
57	MG	1A	3965	1/1	0.90	0.18	52,52,52,52	0
57	MG	1A	3750	1/1	0.90	0.07	59,59,59,59	0
57	MG	2A	3129	1/1	0.90	0.28	45,45,45,45	0
57	MG	1A	3862	1/1	0.90	0.12	49,49,49,49	0
57	MG	1A	3505	1/1	0.90	0.17	46,46,46,46	0
57	MG	1A	3638	1/1	0.90	0.10	56,56,56,56	0
57	MG	1A	3866	1/1	0.90	0.24	36,36,36,36	0
57	MG	1U	207	1/1	0.90	0.50	35,35,35,35	0
57	MG	1a	1679	1/1	0.90	0.15	67,67,67,67	0
57	MG	2A	3672	1/1	0.90	0.11	55,55,55,55	0
57	MG	2W	202	1/1	0.90	0.48	48,48,48,48	0
57	MG	1A	3753	1/1	0.90	0.10	49,49,49,49	0
57	MG	2A	3674	1/1	0.90	0.16	65,65,65,65	0
57	MG	2g	201	1/1	0.90	0.15	81,81,81,81	0
57	MG	1A	3061	1/1	0.90	0.16	65,65,65,65	0
57	MG	2A	3294	1/1	0.90	0.17	53,53,53,53	0
57	MG	1A	3647	1/1	0.90	0.09	25,25,25,25	0
57	MG	1A	3317	1/1	0.90	0.20	49,49,49,49	0
57	MG	2A	3680	1/1	0.90	0.09	76,76,76,76	0
57	MG	28	101	1/1	0.90	0.15	54,54,54,54	0
57	MG	2A	3681	1/1	0.90	0.13	67,67,67,67	0
57	MG	1A	3583	1/1	0.90	0.14	62,62,62,62	0
57	MG	2A	3158	1/1	0.90	0.24	62,62,62,62	0
57	MG	1A	3772	1/1	0.90	0.15	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3163	1/1	0.90	0.12	42,42,42,42	0
57	MG	1A	3171	1/1	0.90	0.48	41,41,41,41	0
57	MG	2A	3303	1/1	0.90	0.35	53,53,53,53	0
57	MG	2A	3701	1/1	0.90	0.10	61,61,61,61	0
57	MG	2A	3702	1/1	0.90	0.21	70,70,70,70	0
57	MG	1A	3990	1/1	0.90	0.09	42,42,42,42	0
57	MG	1W	202	1/1	0.91	0.33	47,47,47,47	0
57	MG	1X	102	1/1	0.91	0.13	26,26,26,26	0
57	MG	2A	3090	1/1	0.91	0.06	67,67,67,67	0
57	MG	2A	3093	1/1	0.91	0.23	40,40,40,40	0
57	MG	1A	4011	1/1	0.91	0.19	19,19,19,19	0
57	MG	1A	3291	1/1	0.91	0.14	45,45,45,45	0
57	MG	2A	3749	1/1	0.91	0.13	67,67,67,67	0
57	MG	1A	3680	1/1	0.91	0.20	16,16,16,16	0
57	MG	1A	3120	1/1	0.91	0.14	36,36,36,36	0
57	MG	2A	3237	1/1	0.91	0.31	52,52,52,52	0
57	MG	2A	3238	1/1	0.91	0.45	63,63,63,63	0
57	MG	2A	3102	1/1	0.91	0.20	77,77,77,77	0
57	MG	1A	4020	1/1	0.91	0.08	50,50,50,50	0
57	MG	2A	3241	1/1	0.91	0.22	71,71,71,71	0
57	MG	2A	3768	1/1	0.91	0.13	51,51,51,51	0
57	MG	1B	203	1/1	0.91	0.16	34,34,34,34	0
57	MG	2A	3778	1/1	0.91	0.14	62,62,62,62	0
57	MG	1A	3545	1/1	0.91	0.22	44,44,44,44	0
57	MG	2A	3554	1/1	0.91	0.14	44,44,44,44	0
57	MG	1A	3367	1/1	0.91	0.25	44,44,44,44	0
57	MG	2A	3115	1/1	0.91	0.14	34,34,34,34	0
57	MG	1A	3865	1/1	0.91	0.14	54,54,54,54	0
57	MG	2A	3251	1/1	0.91	0.13	64,64,64,64	0
57	MG	1A	3017	1/1	0.91	0.28	57,57,57,57	0
57	MG	1A	4026	1/1	0.91	0.10	45,45,45,45	0
57	MG	2A	3792	1/1	0.91	0.16	86,86,86,86	0
57	MG	2A	3572	1/1	0.91	0.18	52,52,52,52	0
57	MG	1A	3320	1/1	0.91	0.15	44,44,44,44	0
57	MG	1A	3785	1/1	0.91	0.23	31,31,31,31	0
57	MG	2A	3800	1/1	0.91	0.08	44,44,44,44	0
57	MG	2A	3256	1/1	0.91	0.22	61,61,61,61	0
57	MG	1a	1701	1/1	0.91	0.21	47,47,47,47	0
57	MG	1A	3148	1/1	0.91	0.80	37,37,37,37	0
57	MG	2A	3584	1/1	0.91	0.18	61,61,61,61	0
57	MG	2A	3261	1/1	0.91	0.16	72,72,72,72	0
57	MG	1A	3788	1/1	0.91	0.17	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3879	1/1	0.91	0.21	51,51,51,51	0
57	MG	2a	1677	1/1	0.91	0.22	66,66,66,66	0
57	MG	1A	3447	1/1	0.91	0.26	62,62,62,62	0
57	MG	1A	3412	1/1	0.91	0.23	55,55,55,55	0
57	MG	1A	3374	1/1	0.91	0.59	45,45,45,45	0
57	MG	2A	3600	1/1	0.91	0.14	65,65,65,65	0
57	MG	2A	3138	1/1	0.91	0.12	39,39,39,39	0
57	MG	1A	3326	1/1	0.91	0.19	30,30,30,30	0
57	MG	2A	3141	1/1	0.91	0.14	58,58,58,58	0
57	MG	1A	3377	1/1	0.91	0.18	45,45,45,45	0
57	MG	2A	3391	1/1	0.91	0.23	61,61,61,61	0
57	MG	1A	3379	1/1	0.91	0.40	47,47,47,47	0
57	MG	2a	1696	1/1	0.91	0.17	61,61,61,61	0
57	MG	2A	3839	1/1	0.91	0.34	69,69,69,69	0
57	MG	2A	3393	1/1	0.91	0.78	63,63,63,63	0
57	MG	1A	3328	1/1	0.91	0.23	61,61,61,61	0
57	MG	2a	1702	1/1	0.91	0.11	80,80,80,80	0
57	MG	2A	3276	1/1	0.91	0.26	49,49,49,49	0
57	MG	2A	3618	1/1	0.91	0.11	32,32,32,32	0
57	MG	1A	3381	1/1	0.91	0.31	61,61,61,61	0
57	MG	1a	1616	1/1	0.91	0.18	58,58,58,58	0
57	MG	2A	3850	1/1	0.91	0.09	57,57,57,57	0
57	MG	2A	3851	1/1	0.91	0.26	64,64,64,64	0
57	MG	2A	3280	1/1	0.91	0.19	65,65,65,65	0
57	MG	1A	3974	1/1	0.91	0.15	22,22,22,22	0
57	MG	1A	3975	1/1	0.91	0.12	60,60,60,60	0
57	MG	1a	1726	1/1	0.91	0.28	43,43,43,43	0
57	MG	2A	3162	1/1	0.91	0.11	58,58,58,58	0
57	MG	2a	1719	1/1	0.91	0.10	64,64,64,64	0
57	MG	2A	3029	1/1	0.91	0.25	55,55,55,55	0
57	MG	2B	202	1/1	0.91	0.31	76,76,76,76	0
57	MG	2B	203	1/1	0.91	0.10	71,71,71,71	0
57	MG	2a	1724	1/1	0.91	0.17	67,67,67,67	0
57	MG	2a	1725	1/1	0.91	0.24	78,78,78,78	0
57	MG	1A	4050	1/1	0.91	0.19	46,46,46,46	0
57	MG	1A	3349	1/1	0.91	0.10	55,55,55,55	0
57	MG	1A	3978	1/1	0.91	0.16	25,25,25,25	0
57	MG	2a	1732	1/1	0.91	0.28	64,64,64,64	0
57	MG	1A	3384	1/1	0.91	0.64	43,43,43,43	0
57	MG	2A	3036	1/1	0.91	0.18	57,57,57,57	0
57	MG	2A	3171	1/1	0.91	0.38	56,56,56,56	0
57	MG	1A	4055	1/1	0.91	0.13	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3426	1/1	0.91	0.18	59,59,59,59	0
57	MG	2A	3040	1/1	0.91	0.23	54,54,54,54	0
57	MG	2A	3657	1/1	0.91	0.14	68,68,68,68	0
57	MG	2A	3658	1/1	0.91	0.10	27,27,27,27	0
57	MG	1A	3820	1/1	0.91	0.15	51,51,51,51	0
57	MG	1A	3983	1/1	0.91	0.11	59,59,59,59	0
57	MG	1a	1748	1/1	0.91	0.10	66,66,66,66	0
57	MG	2D	306	1/1	0.91	0.45	54,54,54,54	0
57	MG	2D	307	1/1	0.91	0.08	62,62,62,62	0
57	MG	2A	3301	1/1	0.91	0.09	67,67,67,67	0
57	MG	1a	1749	1/1	0.91	0.14	53,53,53,53	0
57	MG	2A	3667	1/1	0.91	0.14	49,49,49,49	0
57	MG	2A	3183	1/1	0.91	0.24	55,55,55,55	0
57	MG	2A	3046	1/1	0.91	0.10	56,56,56,56	0
57	MG	1A	4060	1/1	0.91	0.14	15,15,15,15	0
57	MG	2A	3307	1/1	0.91	0.09	75,75,75,75	0
57	MG	1A	3904	1/1	0.91	0.10	48,48,48,48	0
57	MG	2A	3191	1/1	0.91	0.16	63,63,63,63	0
57	MG	1A	3469	1/1	0.91	0.13	65,65,65,65	0
57	MG	2A	3458	1/1	0.91	0.32	46,46,46,46	0
57	MG	2a	1780	1/1	0.91	0.10	61,61,61,61	0
57	MG	1A	3385	1/1	0.91	0.13	44,44,44,44	0
57	MG	1a	1639	1/1	0.91	0.20	65,65,65,65	0
57	MG	1O	202	1/1	0.91	0.33	51,51,51,51	0
57	MG	2a	1786	1/1	0.91	0.14	72,72,72,72	0
57	MG	1A	3098	1/1	0.91	0.19	41,41,41,41	0
57	MG	2R	201	1/1	0.91	0.27	68,68,68,68	0
57	MG	2A	3056	1/1	0.91	0.11	64,64,64,64	0
57	MG	1a	1773	1/1	0.91	0.16	70,70,70,70	0
57	MG	2T	3502	1/1	0.91	0.27	59,59,59,59	0
57	MG	1A	3653	1/1	0.91	0.17	24,24,24,24	0
57	MG	2A	3698	1/1	0.91	0.12	24,24,24,24	0
57	MG	2A	3474	1/1	0.91	0.18	54,54,54,54	0
57	MG	1A	3841	1/1	0.91	0.13	39,39,39,39	0
57	MG	1A	3742	1/1	0.91	0.27	43,43,43,43	0
57	MG	2A	3205	1/1	0.91	0.10	67,67,67,67	0
57	MG	2I	101	1/1	0.91	0.15	63,63,63,63	0
57	MG	2a	1813	1/1	0.91	0.07	83,83,83,83	0
57	MG	1R	204	1/1	0.91	0.33	37,37,37,37	0
57	MG	23	101	1/1	0.91	0.85	64,64,64,64	0
57	MG	1a	1654	1/1	0.91	0.13	48,48,48,48	0
57	MG	1A	3157	1/1	0.91	0.21	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2a	1823	1/1	0.91	0.11	78,78,78,78	0
57	MG	1A	3007	1/1	0.91	0.17	35,35,35,35	0
57	MG	1A	4000	1/1	0.91	0.12	48,48,48,48	0
57	MG	2A	3712	1/1	0.91	0.05	56,56,56,56	0
57	MG	1a	1662	1/1	0.91	0.12	56,56,56,56	0
57	MG	2A	3715	1/1	0.91	0.13	72,72,72,72	0
57	MG	2A	3074	1/1	0.91	0.20	47,47,47,47	0
57	MG	1A	3362	1/1	0.91	0.20	49,49,49,49	0
57	MG	1A	3108	1/1	0.91	0.54	37,37,37,37	0
57	MG	2a	1606	1/1	0.91	0.21	77,77,77,77	0
57	MG	2A	3721	1/1	0.91	0.11	63,63,63,63	0
57	MG	1A	4085	1/1	0.91	0.12	72,72,72,72	0
57	MG	1A	3277	1/1	0.91	0.19	49,49,49,49	0
57	MG	1A	3401	1/1	0.91	0.46	42,42,42,42	0
57	MG	2A	3223	1/1	0.91	0.31	50,50,50,50	0
57	MG	1V	202	1/1	0.91	0.37	35,35,35,35	0
57	MG	2A	3507	1/1	0.91	0.21	57,57,57,57	0
57	MG	2A	3509	1/1	0.91	0.13	46,46,46,46	0
57	MG	1a	1671	1/1	0.91	0.08	62,62,62,62	0
57	MG	1V	205	1/1	0.91	0.28	51,51,51,51	0
57	MG	1A	3794	1/1	0.92	0.12	37,37,37,37	0
57	MG	2A	3279	1/1	0.92	0.39	62,62,62,62	0
57	MG	2A	3699	1/1	0.92	0.07	64,64,64,64	0
57	MG	1A	3925	1/1	0.92	0.14	39,39,39,39	0
57	MG	1a	1824	1/1	0.92	0.06	54,54,54,54	0
57	MG	1a	1644	1/1	0.92	0.09	69,69,69,69	0
57	MG	2A	3440	1/1	0.92	0.30	59,59,59,59	0
57	MG	1A	3797	1/1	0.92	0.15	36,36,36,36	0
57	MG	2a	1613	1/1	0.92	0.20	57,57,57,57	0
57	MG	1a	1646	1/1	0.92	0.36	62,62,62,62	0
57	MG	1A	3676	1/1	0.92	0.19	35,35,35,35	0
57	MG	2a	1616	1/1	0.92	0.17	71,71,71,71	0
57	MG	2A	3286	1/1	0.92	0.14	63,63,63,63	0
57	MG	1A	3929	1/1	0.92	0.17	22,22,22,22	0
57	MG	1A	4035	1/1	0.92	0.13	44,44,44,44	0
57	MG	1E	312	1/1	0.92	0.19	25,25,25,25	0
57	MG	2A	3714	1/1	0.92	0.13	41,41,41,41	0
57	MG	1n	102	1/1	0.92	0.08	62,62,62,62	0
57	MG	1A	3288	1/1	0.92	0.09	50,50,50,50	0
57	MG	1t	201	1/1	0.92	0.11	57,57,57,57	0
57	MG	2A	3146	1/1	0.92	0.33	48,48,48,48	0
57	MG	1A	3456	1/1	0.92	0.18	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3470	1/1	0.92	0.08	56,56,56,56	0
57	MG	1A	3348	1/1	0.92	0.33	45,45,45,45	0
57	MG	2a	1632	1/1	0.92	0.25	62,62,62,62	0
57	MG	2a	1633	1/1	0.92	0.28	69,69,69,69	0
57	MG	2A	3728	1/1	0.92	0.14	49,49,49,49	0
57	MG	2A	3151	1/1	0.92	0.11	57,57,57,57	0
57	MG	2A	3153	1/1	0.92	0.17	56,56,56,56	0
57	MG	2A	3475	1/1	0.92	0.18	61,61,61,61	0
57	MG	1E	316	1/1	0.92	0.07	41,41,41,41	0
57	MG	2A	3155	1/1	0.92	0.27	65,65,65,65	0
57	MG	2A	3480	1/1	0.92	0.10	60,60,60,60	0
57	MG	1A	3682	1/1	0.92	0.16	43,43,43,43	0
57	MG	1w	106	1/1	0.92	0.21	71,71,71,71	0
57	MG	2A	3484	1/1	0.92	0.27	67,67,67,67	0
57	MG	1F	313	1/1	0.92	0.17	36,36,36,36	0
57	MG	1A	3941	1/1	0.92	0.10	49,49,49,49	0
57	MG	1G	202	1/1	0.92	0.21	55,55,55,55	0
57	MG	2A	3309	1/1	0.92	0.66	62,62,62,62	0
57	MG	1A	3815	1/1	0.92	0.27	21,21,21,21	0
57	MG	2a	1650	1/1	0.92	0.09	69,69,69,69	0
57	MG	2A	3750	1/1	0.92	0.14	74,74,74,74	0
57	MG	1N	203	1/1	0.92	0.15	40,40,40,40	0
57	MG	2a	1654	1/1	0.92	0.24	85,85,85,85	0
57	MG	2A	3168	1/1	0.92	0.14	63,63,63,63	0
57	MG	2A	3313	1/1	0.92	0.15	46,46,46,46	0
57	MG	1A	3290	1/1	0.92	0.18	36,36,36,36	0
57	MG	2A	3761	1/1	0.92	0.12	36,36,36,36	0
57	MG	2A	3501	1/1	0.92	0.07	64,64,64,64	0
57	MG	1A	3322	1/1	0.92	0.17	54,54,54,54	0
57	MG	1A	3462	1/1	0.92	0.36	44,44,44,44	0
57	MG	1A	3689	1/1	0.92	0.12	42,42,42,42	0
57	MG	1A	3515	1/1	0.92	0.12	49,49,49,49	0
57	MG	1A	3698	1/1	0.92	0.13	51,51,51,51	0
57	MG	2A	3001	1/1	0.92	0.18	59,59,59,59	0
57	MG	2A	3512	1/1	0.92	0.06	65,65,65,65	0
57	MG	2A	3002	1/1	0.92	0.32	58,58,58,58	0
57	MG	1A	3516	1/1	0.92	0.47	52,52,52,52	0
57	MG	1A	3602	1/1	0.92	0.33	46,46,46,46	0
57	MG	1A	3059	1/1	0.92	0.33	57,57,57,57	0
57	MG	1A	3518	1/1	0.92	0.24	66,66,66,66	0
57	MG	1A	3243	1/1	0.92	0.46	42,42,42,42	0
57	MG	2a	1685	1/1	0.92	0.33	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3330	1/1	0.92	0.12	59,59,59,59	0
57	MG	2a	1690	1/1	0.92	0.14	52,52,52,52	0
57	MG	1A	3423	1/1	0.92	0.08	57,57,57,57	0
57	MG	1A	3361	1/1	0.92	0.10	57,57,57,57	0
57	MG	1A	3852	1/1	0.92	0.10	47,47,47,47	0
57	MG	1A	3715	1/1	0.92	0.20	28,28,28,28	0
57	MG	1A	3052	1/1	0.92	0.11	40,40,40,40	0
57	MG	1A	4067	1/1	0.92	0.14	15,15,15,15	0
57	MG	2a	1698	1/1	0.92	0.18	64,64,64,64	0
57	MG	1V	206	1/1	0.92	0.23	54,54,54,54	0
57	MG	1a	1703	1/1	0.92	0.21	48,48,48,48	0
57	MG	2A	3340	1/1	0.92	0.14	53,53,53,53	0
57	MG	2A	3200	1/1	0.92	0.12	50,50,50,50	0
57	MG	2A	3813	1/1	0.92	0.07	47,47,47,47	0
57	MG	2A	3815	1/1	0.92	0.16	39,39,39,39	0
57	MG	1A	3855	1/1	0.92	0.20	51,51,51,51	0
57	MG	1A	3145	1/1	0.92	0.21	28,28,28,28	0
57	MG	1Y	201	1/1	0.92	0.21	52,52,52,52	0
57	MG	2a	1712	1/1	0.92	0.15	61,61,61,61	0
57	MG	2A	3560	1/1	0.92	0.14	35,35,35,35	0
57	MG	1a	1708	1/1	0.92	0.20	70,70,70,70	0
57	MG	1A	3428	1/1	0.92	0.30	57,57,57,57	0
57	MG	1A	3726	1/1	0.92	0.19	43,43,43,43	0
57	MG	2A	3044	1/1	0.92	0.25	55,55,55,55	0
57	MG	2A	3834	1/1	0.92	0.13	28,28,28,28	0
57	MG	1A	4074	1/1	0.92	0.21	39,39,39,39	0
57	MG	2A	3573	1/1	0.92	0.14	50,50,50,50	0
57	MG	1A	3727	1/1	0.92	0.12	41,41,41,41	0
57	MG	1A	3475	1/1	0.92	0.21	47,47,47,47	0
57	MG	1A	3980	1/1	0.92	0.14	47,47,47,47	0
57	MG	1A	3298	1/1	0.92	0.09	58,58,58,58	0
57	MG	1a	1720	1/1	0.92	0.09	65,65,65,65	0
57	MG	1A	4083	1/1	0.92	0.31	40,40,40,40	0
57	MG	2A	3358	1/1	0.92	0.10	61,61,61,61	0
57	MG	2A	3589	1/1	0.92	0.08	44,44,44,44	0
57	MG	2A	3217	1/1	0.92	0.10	60,60,60,60	0
57	MG	2A	3592	1/1	0.92	0.24	64,64,64,64	0
57	MG	1A	3538	1/1	0.92	0.41	47,47,47,47	0
57	MG	1a	1724	1/1	0.92	0.15	53,53,53,53	0
57	MG	2A	3221	1/1	0.92	0.10	57,57,57,57	0
57	MG	15	104	1/1	0.92	0.21	33,33,33,33	0
57	MG	1A	3225	1/1	0.92	0.14	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	4089	1/1	0.92	0.15	47,47,47,47	0
57	MG	2A	3061	1/1	0.92	0.13	45,45,45,45	0
57	MG	17	104	1/1	0.92	0.16	52,52,52,52	0
57	MG	2A	3606	1/1	0.92	0.12	65,65,65,65	0
57	MG	2a	1758	1/1	0.92	0.09	62,62,62,62	0
57	MG	1A	3226	1/1	0.92	0.22	51,51,51,51	0
57	MG	1A	3481	1/1	0.92	0.17	49,49,49,49	0
57	MG	1A	3625	1/1	0.92	0.11	47,47,47,47	0
57	MG	2a	1764	1/1	0.92	0.23	68,68,68,68	0
57	MG	18	105	1/1	0.92	0.21	41,41,41,41	0
57	MG	2a	1766	1/1	0.92	0.09	62,62,62,62	0
57	MG	1A	3434	1/1	0.92	0.16	42,42,42,42	0
57	MG	1a	1746	1/1	0.92	0.22	51,51,51,51	0
57	MG	1A	4095	1/1	0.92	0.15	47,47,47,47	0
57	MG	2a	1770	1/1	0.92	0.06	74,74,74,74	0
57	MG	1A	4096	1/1	0.92	0.28	61,61,61,61	0
57	MG	1A	3074	1/1	0.92	0.18	26,26,26,26	0
57	MG	1A	3547	1/1	0.92	0.36	49,49,49,49	0
57	MG	2A	3624	1/1	0.92	0.13	57,57,57,57	0
57	MG	2A	3382	1/1	0.92	0.13	69,69,69,69	0
57	MG	2D	301	1/1	0.92	0.37	42,42,42,42	0
57	MG	1A	3756	1/1	0.92	0.11	48,48,48,48	0
57	MG	2D	305	1/1	0.92	0.71	44,44,44,44	0
57	MG	1B	204	1/1	0.92	0.21	63,63,63,63	0
57	MG	1A	3189	1/1	0.92	0.18	40,40,40,40	0
57	MG	1A	3885	1/1	0.92	0.14	35,35,35,35	0
57	MG	2A	3634	1/1	0.92	0.19	52,52,52,52	0
57	MG	1A	3405	1/1	0.92	0.15	34,34,34,34	0
57	MG	2a	1795	1/1	0.92	0.14	62,62,62,62	0
57	MG	1a	1772	1/1	0.92	0.08	54,54,54,54	0
57	MG	2a	1798	1/1	0.92	0.15	70,70,70,70	0
57	MG	1A	3637	1/1	0.92	0.18	31,31,31,31	0
57	MG	2a	1800	1/1	0.92	0.14	77,77,77,77	0
57	MG	1a	1774	1/1	0.92	0.15	70,70,70,70	0
57	MG	1A	3310	1/1	0.92	0.19	38,38,38,38	0
57	MG	1A	3312	1/1	0.92	0.30	53,53,53,53	0
57	MG	1A	3372	1/1	0.92	0.09	59,59,59,59	0
57	MG	2A	3397	1/1	0.92	0.21	43,43,43,43	0
57	MG	1A	3652	1/1	0.92	0.21	63,63,63,63	0
57	MG	2A	3097	1/1	0.92	0.16	64,64,64,64	0
57	MG	2P	202	1/1	0.92	0.12	50,50,50,50	0
57	MG	2A	3400	1/1	0.92	0.19	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3443	1/1	0.92	0.14	44,44,44,44	0
57	MG	2A	3404	1/1	0.92	0.28	40,40,40,40	0
57	MG	1A	4015	1/1	0.92	0.10	32,32,32,32	0
57	MG	2a	1822	1/1	0.92	0.21	62,62,62,62	0
57	MG	1A	3783	1/1	0.92	0.23	24,24,24,24	0
57	MG	2a	1825	1/1	0.92	0.19	64,64,64,64	0
57	MG	2A	3103	1/1	0.92	0.18	44,44,44,44	0
57	MG	1a	1800	1/1	0.92	0.13	53,53,53,53	0
57	MG	1a	1801	1/1	0.92	0.07	44,44,44,44	0
57	MG	2i	201	1/1	0.92	0.12	65,65,65,65	0
57	MG	1A	3062	1/1	0.92	0.21	51,51,51,51	0
57	MG	1A	3273	1/1	0.92	0.25	38,38,38,38	0
57	MG	1A	3344	1/1	0.92	0.31	69,69,69,69	0
57	MG	2A	3675	1/1	0.92	0.17	38,38,38,38	0
57	MG	2q	202	1/1	0.92	0.09	76,76,76,76	0
57	MG	2A	3117	1/1	0.92	0.15	70,70,70,70	0
57	MG	1A	3787	1/1	0.92	0.20	28,28,28,28	0
57	MG	1A	3040	1/1	0.92	0.29	51,51,51,51	0
57	MG	2w	102	1/1	0.92	0.37	62,62,62,62	0
57	MG	2A	3421	1/1	0.92	0.15	60,60,60,60	0
57	MG	2A	3121	1/1	0.92	0.07	57,57,57,57	0
57	MG	1A	3494	1/1	0.92	0.28	52,52,52,52	0
57	MG	25	104	1/1	0.92	0.21	53,53,53,53	0
57	MG	1B	233	1/1	0.92	0.08	58,58,58,58	0
57	MG	2x	106	1/1	0.92	0.12	59,59,59,59	0
57	MG	1A	3498	1/1	0.92	0.11	43,43,43,43	0
57	MG	2A	3691	1/1	0.92	0.15	54,54,54,54	0
57	MG	2A	3431	1/1	0.92	0.24	49,49,49,49	0
57	MG	2A	3432	1/1	0.92	0.14	66,66,66,66	0
57	MG	1A	3937	1/1	0.93	0.06	34,34,34,34	0
57	MG	1W	207	1/1	0.93	0.21	27,27,27,27	0
57	MG	2A	3243	1/1	0.93	0.24	60,60,60,60	0
57	MG	1A	3938	1/1	0.93	0.11	42,42,42,42	0
57	MG	1A	3699	1/1	0.93	0.12	26,26,26,26	0
57	MG	1A	3155	1/1	0.93	0.22	31,31,31,31	0
57	MG	1A	3397	1/1	0.93	0.27	31,31,31,31	0
57	MG	1A	3238	1/1	0.93	0.14	30,30,30,30	0
57	MG	1A	3018	1/1	0.93	0.15	26,26,26,26	0
57	MG	1A	3035	1/1	0.93	0.08	44,44,44,44	0
57	MG	1A	3060	1/1	0.93	0.23	30,30,30,30	0
57	MG	2A	3425	1/1	0.93	0.28	63,63,63,63	0
57	MG	2A	3688	1/1	0.93	0.09	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3442	1/1	0.93	0.46	35,35,35,35	0
57	MG	1A	3953	1/1	0.93	0.14	29,29,29,29	0
57	MG	2A	3083	1/1	0.93	0.28	55,55,55,55	0
57	MG	1A	3954	1/1	0.93	0.18	40,40,40,40	0
57	MG	1A	3957	1/1	0.93	0.08	38,38,38,38	0
57	MG	1a	1752	1/1	0.93	0.13	34,34,34,34	0
57	MG	2A	3088	1/1	0.93	0.31	52,52,52,52	0
57	MG	15	107	1/1	0.93	0.15	54,54,54,54	0
57	MG	1a	1756	1/1	0.93	0.22	64,64,64,64	0
57	MG	1A	3099	1/1	0.93	0.26	65,65,65,65	0
57	MG	1A	3828	1/1	0.93	0.13	26,26,26,26	0
57	MG	1A	3829	1/1	0.93	0.22	46,46,46,46	0
57	MG	2A	3445	1/1	0.93	0.23	66,66,66,66	0
57	MG	2A	3096	1/1	0.93	0.18	45,45,45,45	0
57	MG	1A	3830	1/1	0.93	0.05	57,57,57,57	0
57	MG	1A	3832	1/1	0.93	0.19	63,63,63,63	0
57	MG	2A	3099	1/1	0.93	0.17	65,65,65,65	0
57	MG	1A	3718	1/1	0.93	0.10	54,54,54,54	0
57	MG	1a	1770	1/1	0.93	0.10	48,48,48,48	0
57	MG	1A	3835	1/1	0.93	0.29	26,26,26,26	0
57	MG	2A	3104	1/1	0.93	0.33	52,52,52,52	0
57	MG	19	101	1/1	0.93	0.27	49,49,49,49	0
57	MG	1A	4088	1/1	0.93	0.20	51,51,51,51	0
57	MG	2A	3466	1/1	0.93	0.31	43,43,43,43	0
57	MG	1a	1777	1/1	0.93	0.18	66,66,66,66	0
57	MG	1A	3837	1/1	0.93	0.15	39,39,39,39	0
57	MG	1A	3325	1/1	0.93	0.30	41,41,41,41	0
57	MG	1A	4091	1/1	0.93	0.14	51,51,51,51	0
57	MG	1A	3842	1/1	0.93	0.11	40,40,40,40	0
57	MG	1A	3445	1/1	0.93	0.21	41,41,41,41	0
57	MG	2A	3733	1/1	0.93	0.07	43,43,43,43	0
57	MG	1A	3553	1/1	0.93	0.12	53,53,53,53	0
57	MG	1a	1793	1/1	0.93	0.13	70,70,70,70	0
57	MG	1a	1608	1/1	0.93	0.27	52,52,52,52	0
57	MG	1A	3972	1/1	0.93	0.16	29,29,29,29	0
57	MG	2A	3741	1/1	0.93	0.13	59,59,59,59	0
57	MG	1A	3289	1/1	0.93	0.36	49,49,49,49	0
57	MG	1A	3090	1/1	0.93	0.14	40,40,40,40	0
57	MG	1A	3630	1/1	0.93	0.14	35,35,35,35	0
57	MG	1A	3729	1/1	0.93	0.17	50,50,50,50	0
57	MG	1A	3135	1/1	0.93	0.16	44,44,44,44	0
57	MG	2A	3132	1/1	0.93	0.49	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3133	1/1	0.93	0.20	41,41,41,41	0
57	MG	1a	1622	1/1	0.93	0.34	73,73,73,73	0
57	MG	2A	3135	1/1	0.93	0.14	41,41,41,41	0
57	MG	2A	3304	1/1	0.93	0.12	62,62,62,62	0
57	MG	2A	3754	1/1	0.93	0.37	64,64,64,64	0
57	MG	2A	3499	1/1	0.93	0.13	52,52,52,52	0
57	MG	1a	1810	1/1	0.93	0.12	67,67,67,67	0
57	MG	1A	3330	1/1	0.93	0.18	47,47,47,47	0
57	MG	1A	3102	1/1	0.93	0.16	31,31,31,31	0
57	MG	1A	3294	1/1	0.93	0.25	30,30,30,30	0
57	MG	1a	1627	1/1	0.93	0.16	64,64,64,64	0
57	MG	2A	3767	1/1	0.93	0.07	67,67,67,67	0
57	MG	1A	3639	1/1	0.93	0.22	27,27,27,27	0
57	MG	2A	3506	1/1	0.93	0.12	30,30,30,30	0
57	MG	2A	3770	1/1	0.93	0.12	68,68,68,68	0
57	MG	2a	1686	1/1	0.93	0.09	80,80,80,80	0
57	MG	1A	3743	1/1	0.93	0.06	61,61,61,61	0
57	MG	1A	3560	1/1	0.93	0.35	34,34,34,34	0
57	MG	2A	3782	1/1	0.93	0.23	61,61,61,61	0
57	MG	1A	3180	1/1	0.93	0.20	28,28,28,28	0
57	MG	1A	3648	1/1	0.93	0.15	35,35,35,35	0
57	MG	1A	3651	1/1	0.93	0.23	22,22,22,22	0
57	MG	1A	3754	1/1	0.93	0.35	57,57,57,57	0
57	MG	1A	3569	1/1	0.93	0.48	54,54,54,54	0
57	MG	2A	3788	1/1	0.93	0.24	53,53,53,53	0
57	MG	1A	3296	1/1	0.93	0.29	50,50,50,50	0
57	MG	2A	3790	1/1	0.93	0.19	58,58,58,58	0
57	MG	2A	3522	1/1	0.93	0.11	37,37,37,37	0
57	MG	2A	3156	1/1	0.93	0.18	54,54,54,54	0
57	MG	2A	3157	1/1	0.93	0.41	42,42,42,42	0
57	MG	1A	3760	1/1	0.93	0.20	27,27,27,27	0
57	MG	1B	227	1/1	0.93	0.16	38,38,38,38	0
57	MG	1A	3877	1/1	0.93	0.12	38,38,38,38	0
57	MG	2a	1709	1/1	0.93	0.11	67,67,67,67	0
57	MG	1A	4001	1/1	0.93	0.22	31,31,31,31	0
57	MG	2A	3538	1/1	0.93	0.17	40,40,40,40	0
57	MG	2A	3327	1/1	0.93	0.26	51,51,51,51	0
57	MG	2A	3541	1/1	0.93	0.10	45,45,45,45	0
57	MG	1A	3103	1/1	0.93	0.14	27,27,27,27	0
57	MG	2A	3548	1/1	0.93	0.10	71,71,71,71	0
57	MG	1A	3054	1/1	0.93	0.13	40,40,40,40	0
57	MG	2A	3814	1/1	0.93	0.08	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3660	1/1	0.93	0.17	66,66,66,66	0
57	MG	2a	1721	1/1	0.93	0.35	68,68,68,68	0
57	MG	2A	3816	1/1	0.93	0.21	34,34,34,34	0
57	MG	2A	3551	1/1	0.93	0.17	44,44,44,44	0
57	MG	1A	3769	1/1	0.93	0.10	46,46,46,46	0
57	MG	2A	3822	1/1	0.93	0.12	66,66,66,66	0
57	MG	1B	236	1/1	0.93	0.19	31,31,31,31	0
57	MG	1A	3579	1/1	0.93	0.49	39,39,39,39	0
57	MG	1a	1659	1/1	0.93	0.21	66,66,66,66	0
57	MG	2a	1731	1/1	0.93	0.12	80,80,80,80	0
57	MG	2A	3829	1/1	0.93	0.07	68,68,68,68	0
57	MG	1x	102	1/1	0.93	0.16	52,52,52,52	0
57	MG	2a	1735	1/1	0.93	0.13	70,70,70,70	0
57	MG	2a	1736	1/1	0.93	0.18	66,66,66,66	0
57	MG	2A	3558	1/1	0.93	0.16	51,51,51,51	0
57	MG	1A	3511	1/1	0.93	0.29	52,52,52,52	0
57	MG	2A	3175	1/1	0.93	0.29	68,68,68,68	0
57	MG	2A	3562	1/1	0.93	0.14	47,47,47,47	0
57	MG	1x	104	1/1	0.93	0.11	68,68,68,68	0
57	MG	2A	3565	1/1	0.93	0.09	77,77,77,77	0
57	MG	1A	3465	1/1	0.93	0.19	43,43,43,43	0
57	MG	1A	3888	1/1	0.93	0.22	32,32,32,32	0
57	MG	2a	1749	1/1	0.93	0.14	71,71,71,71	0
57	MG	2a	1751	1/1	0.93	0.10	73,73,73,73	0
57	MG	2A	3180	1/1	0.93	0.11	40,40,40,40	0
57	MG	2A	3181	1/1	0.93	0.11	59,59,59,59	0
57	MG	1A	4018	1/1	0.93	0.21	33,33,33,33	0
57	MG	2A	3844	1/1	0.93	0.36	53,53,53,53	0
57	MG	1A	3777	1/1	0.93	0.19	42,42,42,42	0
57	MG	2A	3185	1/1	0.93	0.32	74,74,74,74	0
57	MG	1A	3893	1/1	0.93	0.14	33,33,33,33	0
57	MG	2A	3581	1/1	0.93	0.09	59,59,59,59	0
57	MG	2A	3852	1/1	0.93	0.11	65,65,65,65	0
57	MG	2A	3582	1/1	0.93	0.12	34,34,34,34	0
57	MG	1A	3780	1/1	0.93	0.13	36,36,36,36	0
57	MG	1A	3896	1/1	0.93	0.17	35,35,35,35	0
57	MG	2A	3859	1/1	0.93	0.07	59,59,59,59	0
57	MG	1A	3781	1/1	0.93	0.18	23,23,23,23	0
57	MG	2A	3586	1/1	0.93	0.08	54,54,54,54	0
57	MG	1A	3672	1/1	0.93	0.20	31,31,31,31	0
57	MG	1F	305	1/1	0.93	0.29	30,30,30,30	0
57	MG	2A	3004	1/1	0.93	0.24	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3195	1/1	0.93	0.11	63,63,63,63	0
57	MG	1A	3220	1/1	0.93	0.24	38,38,38,38	0
57	MG	2A	3006	1/1	0.93	0.13	58,58,58,58	0
57	MG	1A	3674	1/1	0.93	0.16	38,38,38,38	0
57	MG	1A	3147	1/1	0.93	0.17	30,30,30,30	0
57	MG	2a	1785	1/1	0.93	0.08	66,66,66,66	0
57	MG	1A	3184	1/1	0.93	0.12	66,66,66,66	0
57	MG	2a	1787	1/1	0.93	0.11	82,82,82,82	0
57	MG	1A	3186	1/1	0.93	0.17	45,45,45,45	0
57	MG	2A	3019	1/1	0.93	0.18	38,38,38,38	0
57	MG	2a	1792	1/1	0.93	0.12	74,74,74,74	0
57	MG	2A	3605	1/1	0.93	0.24	68,68,68,68	0
57	MG	2A	3020	1/1	0.93	0.12	55,55,55,55	0
57	MG	2A	3022	1/1	0.93	0.41	45,45,45,45	0
57	MG	1N	201	1/1	0.93	0.21	56,56,56,56	0
57	MG	1N	202	1/1	0.93	0.45	43,43,43,43	0
57	MG	1A	3910	1/1	0.93	0.12	21,21,21,21	0
57	MG	2D	302	1/1	0.93	0.10	56,56,56,56	0
57	MG	2A	3372	1/1	0.93	0.16	69,69,69,69	0
57	MG	1a	1687	1/1	0.93	0.10	72,72,72,72	0
57	MG	2A	3615	1/1	0.93	0.15	60,60,60,60	0
57	MG	2a	1807	1/1	0.93	0.23	56,56,56,56	0
57	MG	1A	4034	1/1	0.93	0.08	44,44,44,44	0
57	MG	1A	3911	1/1	0.93	0.20	75,75,75,75	0
57	MG	1A	3118	1/1	0.93	0.21	35,35,35,35	0
57	MG	1A	3601	1/1	0.93	0.28	67,67,67,67	0
57	MG	1A	3915	1/1	0.93	0.12	32,32,32,32	0
57	MG	2a	1815	1/1	0.93	0.09	67,67,67,67	0
57	MG	1A	3791	1/1	0.93	0.18	21,21,21,21	0
57	MG	1P	206	1/1	0.93	0.32	49,49,49,49	0
57	MG	1Q	202	1/1	0.93	0.18	30,30,30,30	0
57	MG	1Q	203	1/1	0.93	0.19	40,40,40,40	0
57	MG	1Q	204	1/1	0.93	0.20	61,61,61,61	0
57	MG	2A	3222	1/1	0.93	0.28	41,41,41,41	0
57	MG	1a	1704	1/1	0.93	0.24	58,58,58,58	0
57	MG	2A	3637	1/1	0.93	0.15	49,49,49,49	0
57	MG	2d	302	1/1	0.93	0.08	68,68,68,68	0
57	MG	2e	201	1/1	0.93	0.13	74,74,74,74	0
57	MG	1A	3917	1/1	0.93	0.29	53,53,53,53	0
57	MG	1A	3119	1/1	0.93	0.19	45,45,45,45	0
57	MG	2A	3643	1/1	0.93	0.19	39,39,39,39	0
57	MG	2A	3226	1/1	0.93	0.40	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2l	202	1/1	0.93	0.17	74,74,74,74	0
57	MG	1A	3685	1/1	0.93	0.16	27,27,27,27	0
57	MG	1A	3313	1/1	0.93	0.33	49,49,49,49	0
57	MG	1A	3234	1/1	0.93	0.15	55,55,55,55	0
57	MG	1A	4047	1/1	0.93	0.15	25,25,25,25	0
57	MG	1A	3799	1/1	0.93	0.34	58,58,58,58	0
57	MG	2v	102	1/1	0.93	0.09	61,61,61,61	0
57	MG	2A	3656	1/1	0.93	0.15	55,55,55,55	0
57	MG	1A	3388	1/1	0.93	0.15	58,58,58,58	0
57	MG	2X	101	1/1	0.93	0.37	65,65,65,65	0
57	MG	2w	104	1/1	0.93	0.19	72,72,72,72	0
57	MG	2x	101	1/1	0.93	0.16	49,49,49,49	0
57	MG	1A	3932	1/1	0.93	0.12	33,33,33,33	0
57	MG	1a	1715	1/1	0.93	0.35	63,63,63,63	0
57	MG	1A	3804	1/1	0.93	0.05	45,45,45,45	0
57	MG	1A	3351	1/1	0.93	0.24	39,39,39,39	0
57	MG	2A	3664	1/1	0.93	0.19	60,60,60,60	0
57	MG	1a	1719	1/1	0.93	0.10	62,62,62,62	0
57	MG	1A	3353	1/1	0.93	0.12	36,36,36,36	0
57	MG	1V	207	1/1	0.93	0.21	52,52,52,52	0
57	MG	25	102	1/1	0.93	0.38	50,50,50,50	0
59	ZN	26	102	1/1	0.93	0.20	64,64,64,64	0
59	ZN	2n	501	1/1	0.93	0.10	91,91,91,91	0
57	MG	1a	1641	1/1	0.94	0.25	52,52,52,52	0
57	MG	2A	3187	1/1	0.94	0.22	70,70,70,70	0
57	MG	1A	3503	1/1	0.94	0.33	34,34,34,34	0
57	MG	2X	102	1/1	0.94	0.14	47,47,47,47	0
57	MG	1A	3708	1/1	0.94	0.16	19,19,19,19	0
57	MG	2A	3642	1/1	0.94	0.09	73,73,73,73	0
57	MG	1A	3056	1/1	0.94	0.25	37,37,37,37	0
57	MG	1A	3848	1/1	0.94	0.21	53,53,53,53	0
57	MG	1A	3599	1/1	0.94	0.37	64,64,64,64	0
57	MG	1A	3237	1/1	0.94	0.35	30,30,30,30	0
57	MG	1a	1648	1/1	0.94	0.13	52,52,52,52	0
57	MG	1a	1649	1/1	0.94	0.11	49,49,49,49	0
57	MG	1A	3153	1/1	0.94	0.11	31,31,31,31	0
57	MG	1B	232	1/1	0.94	0.12	59,59,59,59	0
57	MG	1a	1656	1/1	0.94	0.15	66,66,66,66	0
57	MG	27	101	1/1	0.94	0.17	61,61,61,61	0
57	MG	1A	3988	1/1	0.94	0.09	63,63,63,63	0
57	MG	2A	3201	1/1	0.94	0.13	66,66,66,66	0
57	MG	1A	3199	1/1	0.94	0.34	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3661	1/1	0.94	0.09	64,64,64,64	0
57	MG	2a	1602	1/1	0.94	0.28	60,60,60,60	0
57	MG	1A	3076	1/1	0.94	0.20	42,42,42,42	0
57	MG	1A	3605	1/1	0.94	0.30	64,64,64,64	0
57	MG	1A	3340	1/1	0.94	0.40	57,57,57,57	0
57	MG	2A	3206	1/1	0.94	0.40	67,67,67,67	0
57	MG	1A	3608	1/1	0.94	0.16	35,35,35,35	0
57	MG	2A	3011	1/1	0.94	0.10	50,50,50,50	0
57	MG	2a	1609	1/1	0.94	0.20	75,75,75,75	0
57	MG	2a	1610	1/1	0.94	0.13	67,67,67,67	0
57	MG	1E	302	1/1	0.94	0.45	45,45,45,45	0
57	MG	1A	3063	1/1	0.94	0.29	46,46,46,46	0
57	MG	1A	3998	1/1	0.94	0.21	43,43,43,43	0
57	MG	1A	3159	1/1	0.94	0.16	31,31,31,31	0
57	MG	2A	3402	1/1	0.94	0.21	62,62,62,62	0
57	MG	1A	3128	1/1	0.94	0.28	56,56,56,56	0
57	MG	1A	3519	1/1	0.94	0.20	29,29,29,29	0
57	MG	1A	3731	1/1	0.94	0.08	59,59,59,59	0
57	MG	1A	3453	1/1	0.94	0.42	41,41,41,41	0
57	MG	1A	3868	1/1	0.94	0.18	36,36,36,36	0
57	MG	2A	3682	1/1	0.94	0.10	61,61,61,61	0
57	MG	1F	302	1/1	0.94	0.17	25,25,25,25	0
57	MG	2A	3685	1/1	0.94	0.09	48,48,48,48	0
57	MG	2A	3686	1/1	0.94	0.10	70,70,70,70	0
57	MG	1A	3129	1/1	0.94	0.20	31,31,31,31	0
57	MG	1A	3004	1/1	0.94	0.16	20,20,20,20	0
57	MG	1A	4012	1/1	0.94	0.13	28,28,28,28	0
57	MG	2A	3415	1/1	0.94	0.11	63,63,63,63	0
57	MG	2A	3034	1/1	0.94	0.24	49,49,49,49	0
57	MG	2A	3418	1/1	0.94	0.18	59,59,59,59	0
57	MG	2A	3035	1/1	0.94	0.14	37,37,37,37	0
57	MG	1A	3871	1/1	0.94	0.18	19,19,19,19	0
57	MG	1G	201	1/1	0.94	0.22	35,35,35,35	0
57	MG	1a	1686	1/1	0.94	0.21	48,48,48,48	0
57	MG	1A	3873	1/1	0.94	0.12	44,44,44,44	0
57	MG	2A	3703	1/1	0.94	0.12	46,46,46,46	0
57	MG	1a	1688	1/1	0.94	0.21	60,60,60,60	0
57	MG	1A	3738	1/1	0.94	0.22	41,41,41,41	0
57	MG	1A	3741	1/1	0.94	0.10	64,64,64,64	0
57	MG	1A	3211	1/1	0.94	0.13	36,36,36,36	0
57	MG	1A	3878	1/1	0.94	0.18	42,42,42,42	0
57	MG	1A	3403	1/1	0.94	0.29	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3711	1/1	0.94	0.10	45,45,45,45	0
57	MG	2A	3048	1/1	0.94	0.14	42,42,42,42	0
57	MG	2a	1648	1/1	0.94	0.18	73,73,73,73	0
57	MG	1A	3749	1/1	0.94	0.17	21,21,21,21	0
57	MG	1A	3881	1/1	0.94	0.14	22,22,22,22	0
57	MG	2A	3437	1/1	0.94	0.17	60,60,60,60	0
57	MG	1a	1697	1/1	0.94	0.24	43,43,43,43	0
57	MG	1A	3212	1/1	0.94	0.20	43,43,43,43	0
57	MG	2A	3719	1/1	0.94	0.17	36,36,36,36	0
57	MG	1A	3533	1/1	0.94	0.18	53,53,53,53	0
57	MG	2A	3443	1/1	0.94	0.13	53,53,53,53	0
57	MG	2A	3444	1/1	0.94	0.30	44,44,44,44	0
57	MG	1A	3350	1/1	0.94	0.29	54,54,54,54	0
57	MG	1A	3304	1/1	0.94	0.33	44,44,44,44	0
57	MG	2A	3447	1/1	0.94	0.13	48,48,48,48	0
57	MG	1A	3352	1/1	0.94	0.29	37,37,37,37	0
57	MG	1A	3755	1/1	0.94	0.10	51,51,51,51	0
57	MG	2A	3453	1/1	0.94	0.26	71,71,71,71	0
57	MG	2A	3246	1/1	0.94	0.11	60,60,60,60	0
57	MG	2A	3248	1/1	0.94	0.39	61,61,61,61	0
57	MG	2A	3059	1/1	0.94	0.16	54,54,54,54	0
57	MG	1A	3891	1/1	0.94	0.30	29,29,29,29	0
57	MG	2A	3740	1/1	0.94	0.48	65,65,65,65	0
57	MG	1A	3253	1/1	0.94	0.16	45,45,45,45	0
57	MG	1A	3540	1/1	0.94	0.28	42,42,42,42	0
57	MG	2A	3064	1/1	0.94	0.13	60,60,60,60	0
57	MG	2a	1684	1/1	0.94	0.21	55,55,55,55	0
57	MG	1A	3631	1/1	0.94	0.14	38,38,38,38	0
57	MG	1S	201	1/1	0.94	0.56	41,41,41,41	0
57	MG	1A	3254	1/1	0.94	0.28	52,52,52,52	0
57	MG	2a	1689	1/1	0.94	0.13	79,79,79,79	0
57	MG	1A	3634	1/1	0.94	0.17	32,32,32,32	0
57	MG	1A	3255	1/1	0.94	0.31	49,49,49,49	0
57	MG	1U	202	1/1	0.94	0.27	40,40,40,40	0
57	MG	1A	4041	1/1	0.94	0.22	68,68,68,68	0
57	MG	1A	3768	1/1	0.94	0.15	53,53,53,53	0
57	MG	1U	205	1/1	0.94	0.34	35,35,35,35	0
57	MG	2A	3755	1/1	0.94	0.12	65,65,65,65	0
57	MG	2A	3479	1/1	0.94	0.11	65,65,65,65	0
57	MG	1A	3900	1/1	0.94	0.17	28,28,28,28	0
57	MG	1a	1722	1/1	0.94	0.14	48,48,48,48	0
57	MG	2A	3482	1/1	0.94	0.09	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1U	208	1/1	0.94	0.22	39,39,39,39	0
57	MG	1A	3085	1/1	0.94	0.43	23,23,23,23	0
57	MG	1A	3770	1/1	0.94	0.15	39,39,39,39	0
57	MG	1A	3050	1/1	0.94	0.24	27,27,27,27	0
57	MG	1A	3069	1/1	0.94	0.22	23,23,23,23	0
57	MG	1A	4048	1/1	0.94	0.34	49,49,49,49	0
57	MG	2A	3772	1/1	0.94	0.08	64,64,64,64	0
57	MG	2A	3775	1/1	0.94	0.12	52,52,52,52	0
57	MG	2A	3776	1/1	0.94	0.06	55,55,55,55	0
57	MG	1A	3775	1/1	0.94	0.18	51,51,51,51	0
57	MG	1A	3643	1/1	0.94	0.20	54,54,54,54	0
57	MG	2A	3780	1/1	0.94	0.09	37,37,37,37	0
57	MG	1A	3548	1/1	0.94	0.18	25,25,25,25	0
57	MG	2A	3496	1/1	0.94	0.09	59,59,59,59	0
57	MG	2A	3091	1/1	0.94	0.24	40,40,40,40	0
57	MG	2A	3092	1/1	0.94	0.35	50,50,50,50	0
57	MG	1Z	301	1/1	0.94	0.17	59,59,59,59	0
57	MG	1a	1744	1/1	0.94	0.39	56,56,56,56	0
57	MG	10	101	1/1	0.94	0.18	38,38,38,38	0
57	MG	10	103	1/1	0.94	0.19	37,37,37,37	0
57	MG	1a	1747	1/1	0.94	0.17	60,60,60,60	0
57	MG	1A	3779	1/1	0.94	0.21	20,20,20,20	0
57	MG	10	106	1/1	0.94	0.11	51,51,51,51	0
57	MG	2A	3100	1/1	0.94	0.11	33,33,33,33	0
57	MG	2A	3794	1/1	0.94	0.08	61,61,61,61	0
57	MG	1a	1751	1/1	0.94	0.09	66,66,66,66	0
57	MG	2A	3511	1/1	0.94	0.13	56,56,56,56	0
57	MG	1A	3549	1/1	0.94	0.31	44,44,44,44	0
57	MG	2A	3801	1/1	0.94	0.07	55,55,55,55	0
57	MG	2A	3292	1/1	0.94	0.07	57,57,57,57	0
57	MG	2A	3293	1/1	0.94	0.13	66,66,66,66	0
57	MG	1A	3139	1/1	0.94	0.19	41,41,41,41	0
57	MG	1A	3316	1/1	0.94	0.24	54,54,54,54	0
57	MG	2A	3105	1/1	0.94	0.13	43,43,43,43	0
57	MG	2a	1744	1/1	0.94	0.06	78,78,78,78	0
57	MG	2a	1746	1/1	0.94	0.10	62,62,62,62	0
57	MG	1A	3418	1/1	0.94	0.28	48,48,48,48	0
57	MG	2A	3107	1/1	0.94	0.17	61,61,61,61	0
57	MG	1A	3921	1/1	0.94	0.21	53,53,53,53	0
57	MG	1a	1759	1/1	0.94	0.23	76,76,76,76	0
57	MG	13	102	1/1	0.94	0.22	37,37,37,37	0
57	MG	1A	3012	1/1	0.94	0.11	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3532	1/1	0.94	0.11	46,46,46,46	0
57	MG	2A	3116	1/1	0.94	0.27	45,45,45,45	0
57	MG	2a	1760	1/1	0.94	0.10	48,48,48,48	0
57	MG	1A	4063	1/1	0.94	0.10	42,42,42,42	0
57	MG	2A	3824	1/1	0.94	0.15	50,50,50,50	0
57	MG	1a	1766	1/1	0.94	0.09	52,52,52,52	0
57	MG	13	105	1/1	0.94	0.13	53,53,53,53	0
57	MG	1a	1768	1/1	0.94	0.05	64,64,64,64	0
57	MG	2A	3545	1/1	0.94	0.14	31,31,31,31	0
57	MG	2A	3122	1/1	0.94	0.07	67,67,67,67	0
57	MG	1A	3221	1/1	0.94	0.26	40,40,40,40	0
57	MG	15	101	1/1	0.94	0.38	33,33,33,33	0
57	MG	2A	3125	1/1	0.94	0.12	41,41,41,41	0
57	MG	1A	3106	1/1	0.94	0.17	23,23,23,23	0
57	MG	1A	3659	1/1	0.94	0.21	57,57,57,57	0
57	MG	1A	3321	1/1	0.94	0.22	52,52,52,52	0
57	MG	1A	3664	1/1	0.94	0.10	22,22,22,22	0
57	MG	1a	1779	1/1	0.94	0.13	49,49,49,49	0
57	MG	1a	1780	1/1	0.94	0.11	56,56,56,56	0
57	MG	2a	1781	1/1	0.94	0.17	75,75,75,75	0
57	MG	1A	3223	1/1	0.94	0.12	44,44,44,44	0
57	MG	1A	3107	1/1	0.94	0.27	36,36,36,36	0
57	MG	2A	3320	1/1	0.94	0.08	56,56,56,56	0
57	MG	1A	3667	1/1	0.94	0.21	44,44,44,44	0
57	MG	2A	3848	1/1	0.94	0.21	52,52,52,52	0
57	MG	2A	3849	1/1	0.94	0.12	56,56,56,56	0
57	MG	2A	3322	1/1	0.94	0.19	44,44,44,44	0
57	MG	2a	1790	1/1	0.94	0.20	64,64,64,64	0
57	MG	1a	1786	1/1	0.94	0.07	63,63,63,63	0
57	MG	2A	3567	1/1	0.94	0.09	67,67,67,67	0
57	MG	2A	3136	1/1	0.94	0.15	55,55,55,55	0
57	MG	1A	3668	1/1	0.94	0.15	29,29,29,29	0
57	MG	1A	3371	1/1	0.94	0.22	53,53,53,53	0
57	MG	2a	1797	1/1	0.94	0.20	74,74,74,74	0
57	MG	2A	3139	1/1	0.94	0.12	43,43,43,43	0
57	MG	2A	3860	1/1	0.94	0.09	57,57,57,57	0
57	MG	18	106	1/1	0.94	0.19	47,47,47,47	0
57	MG	2A	3576	1/1	0.94	0.15	28,28,28,28	0
57	MG	1A	3033	1/1	0.94	0.27	25,25,25,25	0
57	MG	1A	3566	1/1	0.94	0.28	31,31,31,31	0
57	MG	1A	3803	1/1	0.94	0.14	33,33,33,33	0
57	MG	1A	3091	1/1	0.94	0.16	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3151	1/1	0.94	0.28	36,36,36,36	0
57	MG	1A	3275	1/1	0.94	0.14	49,49,49,49	0
57	MG	2A	3149	1/1	0.94	0.30	51,51,51,51	0
57	MG	1A	3679	1/1	0.94	0.16	20,20,20,20	0
57	MG	1A	3950	1/1	0.94	0.10	54,54,54,54	0
57	MG	1A	3811	1/1	0.94	0.12	46,46,46,46	0
57	MG	1A	3378	1/1	0.94	0.15	40,40,40,40	0
57	MG	2B	212	1/1	0.94	0.17	73,73,73,73	0
57	MG	2a	1818	1/1	0.94	0.20	61,61,61,61	0
57	MG	2a	1819	1/1	0.94	0.05	82,82,82,82	0
57	MG	2a	1820	1/1	0.94	0.21	67,67,67,67	0
57	MG	2A	3593	1/1	0.94	0.21	55,55,55,55	0
57	MG	2A	3594	1/1	0.94	0.22	55,55,55,55	0
57	MG	1A	3188	1/1	0.94	0.29	41,41,41,41	0
57	MG	1A	3281	1/1	0.94	0.61	42,42,42,42	0
57	MG	1A	3580	1/1	0.94	0.13	34,34,34,34	0
57	MG	1a	1819	1/1	0.94	0.08	62,62,62,62	0
57	MG	1a	1820	1/1	0.94	0.29	61,61,61,61	0
57	MG	1A	3819	1/1	0.94	0.06	48,48,48,48	0
57	MG	2D	304	1/1	0.94	0.11	31,31,31,31	0
57	MG	1A	3581	1/1	0.94	0.21	52,52,52,52	0
57	MG	2A	3603	1/1	0.94	0.14	35,35,35,35	0
57	MG	2A	3164	1/1	0.94	0.10	55,55,55,55	0
57	MG	2I	201	1/1	0.94	0.14	54,54,54,54	0
57	MG	1e	201	1/1	0.94	0.11	70,70,70,70	0
57	MG	1A	3495	1/1	0.94	0.27	49,49,49,49	0
57	MG	1A	3584	1/1	0.94	0.22	35,35,35,35	0
57	MG	1A	3963	1/1	0.94	0.17	39,39,39,39	0
57	MG	1A	3332	1/1	0.94	0.23	51,51,51,51	0
57	MG	1A	3691	1/1	0.94	0.23	22,22,22,22	0
57	MG	1A	3693	1/1	0.94	0.20	19,19,19,19	0
57	MG	1A	3586	1/1	0.94	0.19	51,51,51,51	0
57	MG	1A	3831	1/1	0.94	0.10	57,57,57,57	0
57	MG	2A	3360	1/1	0.94	0.41	48,48,48,48	0
57	MG	1A	3382	1/1	0.94	0.29	57,57,57,57	0
57	MG	2O	201	1/1	0.94	0.18	54,54,54,54	0
57	MG	1A	3833	1/1	0.94	0.15	31,31,31,31	0
57	MG	2A	3621	1/1	0.94	0.07	36,36,36,36	0
57	MG	2Q	201	1/1	0.94	0.07	50,50,50,50	0
57	MG	1a	1634	1/1	0.94	0.15	24,24,24,24	0
57	MG	1A	3589	1/1	0.94	0.24	44,44,44,44	0
58	K	1A	3570	1/1	0.94	0.09	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3179	1/1	0.94	0.23	52,52,52,52	0
57	MG	1A	3590	1/1	0.94	0.23	42,42,42,42	0
57	MG	1A	3285	1/1	0.94	0.20	49,49,49,49	0
57	MG	1a	1638	1/1	0.94	0.17	45,45,45,45	0
57	MG	1A	3840	1/1	0.94	0.11	27,27,27,27	0
57	MG	1A	3501	1/1	0.94	0.16	51,51,51,51	0
57	MG	1N	206	1/1	0.95	0.30	44,44,44,44	0
57	MG	1A	3235	1/1	0.95	0.62	47,47,47,47	0
57	MG	1A	3812	1/1	0.95	0.20	16,16,16,16	0
57	MG	1O	203	1/1	0.95	0.10	50,50,50,50	0
57	MG	1A	3924	1/1	0.95	0.13	48,48,48,48	0
57	MG	1A	3814	1/1	0.95	0.17	27,27,27,27	0
57	MG	1P	202	1/1	0.95	0.16	27,27,27,27	0
57	MG	1A	3459	1/1	0.95	0.13	38,38,38,38	0
57	MG	1A	3327	1/1	0.95	0.16	48,48,48,48	0
57	MG	1a	1672	1/1	0.95	0.25	60,60,60,60	0
57	MG	1A	3928	1/1	0.95	0.16	32,32,32,32	0
57	MG	2A	3161	1/1	0.95	0.23	62,62,62,62	0
57	MG	1A	3701	1/1	0.95	0.18	21,21,21,21	0
57	MG	1A	3931	1/1	0.95	0.18	20,20,20,20	0
57	MG	1A	3461	1/1	0.95	0.53	45,45,45,45	0
57	MG	1R	202	1/1	0.95	0.25	48,48,48,48	0
57	MG	1A	3525	1/1	0.95	0.16	45,45,45,45	0
57	MG	1A	3609	1/1	0.95	0.44	62,62,62,62	0
57	MG	2A	3516	1/1	0.95	0.13	44,44,44,44	0
57	MG	1A	3116	1/1	0.95	0.22	36,36,36,36	0
57	MG	1a	1682	1/1	0.95	0.22	75,75,75,75	0
57	MG	1A	3709	1/1	0.95	0.16	23,23,23,23	0
57	MG	1A	3528	1/1	0.95	0.35	42,42,42,42	0
57	MG	1A	3134	1/1	0.95	0.12	37,37,37,37	0
57	MG	1A	3614	1/1	0.95	0.15	50,50,50,50	0
57	MG	1T	202	1/1	0.95	0.15	59,59,59,59	0
57	MG	2A	3758	1/1	0.95	0.16	66,66,66,66	0
57	MG	2A	3759	1/1	0.95	0.12	57,57,57,57	0
57	MG	2A	3530	1/1	0.95	0.09	52,52,52,52	0
57	MG	1A	4057	1/1	0.95	0.17	38,38,38,38	0
57	MG	2a	1651	1/1	0.95	0.47	63,63,63,63	0
57	MG	1A	3464	1/1	0.95	0.08	56,56,56,56	0
57	MG	2A	3765	1/1	0.95	0.12	68,68,68,68	0
57	MG	2A	3533	1/1	0.95	0.12	47,47,47,47	0
57	MG	2A	3337	1/1	0.95	0.17	61,61,61,61	0
57	MG	2A	3536	1/1	0.95	0.17	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3616	1/1	0.95	0.32	41,41,41,41	0
57	MG	1A	3944	1/1	0.95	0.17	39,39,39,39	0
57	MG	2a	1659	1/1	0.95	0.06	71,71,71,71	0
57	MG	2A	3540	1/1	0.95	0.11	52,52,52,52	0
57	MG	1U	206	1/1	0.95	0.18	27,27,27,27	0
57	MG	1A	3286	1/1	0.95	0.20	47,47,47,47	0
57	MG	2a	1665	1/1	0.95	0.14	61,61,61,61	0
57	MG	2A	3015	1/1	0.95	0.24	42,42,42,42	0
57	MG	1A	3078	1/1	0.95	0.21	25,25,25,25	0
57	MG	1a	1700	1/1	0.95	0.32	59,59,59,59	0
57	MG	1A	3537	1/1	0.95	0.35	30,30,30,30	0
57	MG	1V	203	1/1	0.95	0.15	32,32,32,32	0
57	MG	2a	1674	1/1	0.95	0.15	65,65,65,65	0
57	MG	2a	1675	1/1	0.95	0.11	62,62,62,62	0
57	MG	1V	204	1/1	0.95	0.24	28,28,28,28	0
57	MG	1A	3202	1/1	0.95	0.16	38,38,38,38	0
57	MG	2A	3190	1/1	0.95	0.45	72,72,72,72	0
57	MG	1A	3203	1/1	0.95	0.20	30,30,30,30	0
57	MG	2A	3025	1/1	0.95	0.32	61,61,61,61	0
57	MG	1A	3375	1/1	0.95	0.53	42,42,42,42	0
57	MG	2A	3559	1/1	0.95	0.13	37,37,37,37	0
57	MG	1A	3470	1/1	0.95	0.18	63,63,63,63	0
57	MG	1A	3046	1/1	0.95	0.12	34,34,34,34	0
57	MG	1A	3843	1/1	0.95	0.11	36,36,36,36	0
57	MG	1A	3420	1/1	0.95	0.17	35,35,35,35	0
57	MG	1A	4077	1/1	0.95	0.14	35,35,35,35	0
57	MG	1A	3474	1/1	0.95	0.20	35,35,35,35	0
57	MG	1A	3734	1/1	0.95	0.17	57,57,57,57	0
57	MG	2A	3037	1/1	0.95	0.15	39,39,39,39	0
57	MG	1A	3167	1/1	0.95	0.20	36,36,36,36	0
57	MG	1a	1716	1/1	0.95	0.16	68,68,68,68	0
57	MG	1A	3477	1/1	0.95	0.11	70,70,70,70	0
57	MG	1A	3169	1/1	0.95	0.23	65,65,65,65	0
57	MG	2A	3810	1/1	0.95	0.11	54,54,54,54	0
57	MG	1A	3080	1/1	0.95	0.23	33,33,33,33	0
57	MG	2A	3577	1/1	0.95	0.11	64,64,64,64	0
57	MG	1A	3633	1/1	0.95	0.17	19,19,19,19	0
57	MG	1A	3121	1/1	0.95	0.66	46,46,46,46	0
57	MG	2A	3580	1/1	0.95	0.10	54,54,54,54	0
57	MG	1A	3857	1/1	0.95	0.28	52,52,52,52	0
57	MG	1A	3969	1/1	0.95	0.09	43,43,43,43	0
57	MG	2A	3818	1/1	0.95	0.05	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2a	1710	1/1	0.95	0.14	75,75,75,75	0
57	MG	1A	3744	1/1	0.95	0.08	50,50,50,50	0
57	MG	1A	3048	1/1	0.95	0.19	21,21,21,21	0
57	MG	1A	3173	1/1	0.95	0.12	33,33,33,33	0
57	MG	1A	3174	1/1	0.95	0.38	31,31,31,31	0
57	MG	1A	3215	1/1	0.95	0.13	50,50,50,50	0
57	MG	1a	1729	1/1	0.95	0.20	51,51,51,51	0
57	MG	2A	3591	1/1	0.95	0.07	37,37,37,37	0
57	MG	1a	1730	1/1	0.95	0.20	52,52,52,52	0
57	MG	1a	1733	1/1	0.95	0.22	61,61,61,61	0
57	MG	15	102	1/1	0.95	0.16	32,32,32,32	0
57	MG	1A	3178	1/1	0.95	0.24	18,18,18,18	0
57	MG	1a	1741	1/1	0.95	0.15	58,58,58,58	0
57	MG	15	105	1/1	0.95	0.23	31,31,31,31	0
57	MG	2A	3386	1/1	0.95	0.14	61,61,61,61	0
57	MG	1A	3432	1/1	0.95	0.28	37,37,37,37	0
57	MG	1A	3124	1/1	0.95	0.22	33,33,33,33	0
57	MG	1A	3867	1/1	0.95	0.21	15,15,15,15	0
57	MG	2A	3065	1/1	0.95	0.15	45,45,45,45	0
57	MG	1A	3126	1/1	0.95	0.51	38,38,38,38	0
57	MG	2A	3067	1/1	0.95	0.10	48,48,48,48	0
57	MG	1B	205	1/1	0.95	0.14	39,39,39,39	0
57	MG	1A	3649	1/1	0.95	0.15	15,15,15,15	0
57	MG	1A	3435	1/1	0.95	0.35	44,44,44,44	0
57	MG	1A	3034	1/1	0.95	0.36	34,34,34,34	0
57	MG	1A	3762	1/1	0.95	0.14	14,14,14,14	0
57	MG	1a	1754	1/1	0.95	0.11	39,39,39,39	0
57	MG	1A	3986	1/1	0.95	0.19	59,59,59,59	0
57	MG	2A	3853	1/1	0.95	0.07	63,63,63,63	0
57	MG	1A	3389	1/1	0.95	0.20	55,55,55,55	0
57	MG	2A	3856	1/1	0.95	0.09	48,48,48,48	0
57	MG	2A	3077	1/1	0.95	0.16	25,25,25,25	0
57	MG	2A	3405	1/1	0.95	0.20	50,50,50,50	0
57	MG	2A	3406	1/1	0.95	0.33	50,50,50,50	0
57	MG	2a	1750	1/1	0.95	0.14	82,82,82,82	0
57	MG	1A	3875	1/1	0.95	0.13	48,48,48,48	0
57	MG	1A	3568	1/1	0.95	0.18	48,48,48,48	0
57	MG	1A	3655	1/1	0.95	0.18	36,36,36,36	0
57	MG	1A	3042	1/1	0.95	0.29	29,29,29,29	0
57	MG	1a	1762	1/1	0.95	0.13	38,38,38,38	0
57	MG	1A	3657	1/1	0.95	0.17	21,21,21,21	0
57	MG	1B	224	1/1	0.95	0.17	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3086	1/1	0.95	0.13	47,47,47,47	0
57	MG	1A	3263	1/1	0.95	0.22	66,66,66,66	0
57	MG	1A	3572	1/1	0.95	0.35	32,32,32,32	0
57	MG	2A	3636	1/1	0.95	0.20	36,36,36,36	0
57	MG	1A	3575	1/1	0.95	0.29	31,31,31,31	0
57	MG	1a	1769	1/1	0.95	0.20	34,34,34,34	0
57	MG	1a	1613	1/1	0.95	0.17	67,67,67,67	0
57	MG	1a	1771	1/1	0.95	0.11	53,53,53,53	0
57	MG	1A	3006	1/1	0.95	0.25	65,65,65,65	0
57	MG	1A	3396	1/1	0.95	0.33	29,29,29,29	0
57	MG	1A	4003	1/1	0.95	0.24	32,32,32,32	0
57	MG	2a	1773	1/1	0.95	0.12	61,61,61,61	0
57	MG	2a	1775	1/1	0.95	0.12	58,58,58,58	0
57	MG	2A	3646	1/1	0.95	0.16	64,64,64,64	0
57	MG	2A	3647	1/1	0.95	0.12	62,62,62,62	0
57	MG	2A	3428	1/1	0.95	0.11	56,56,56,56	0
57	MG	1A	3497	1/1	0.95	0.29	44,44,44,44	0
57	MG	2A	3260	1/1	0.95	0.14	65,65,65,65	0
57	MG	1a	1620	1/1	0.95	0.21	47,47,47,47	0
57	MG	1A	3185	1/1	0.95	0.17	36,36,36,36	0
57	MG	1A	3154	1/1	0.95	0.12	34,34,34,34	0
57	MG	1A	3400	1/1	0.95	0.71	46,46,46,46	0
57	MG	2A	3265	1/1	0.95	0.10	67,67,67,67	0
57	MG	1A	4010	1/1	0.95	0.19	24,24,24,24	0
57	MG	1D	306	1/1	0.95	0.16	30,30,30,30	0
57	MG	1a	1784	1/1	0.95	0.11	54,54,54,54	0
57	MG	1A	3267	1/1	0.95	0.30	35,35,35,35	0
57	MG	2F	301	1/1	0.95	0.26	38,38,38,38	0
57	MG	2a	1793	1/1	0.95	0.28	66,66,66,66	0
57	MG	1A	3110	1/1	0.95	0.16	39,39,39,39	0
57	MG	1A	3675	1/1	0.95	0.20	55,55,55,55	0
57	MG	1a	1631	1/1	0.95	0.15	70,70,70,70	0
57	MG	1A	3132	1/1	0.95	0.14	34,34,34,34	0
57	MG	2A	3670	1/1	0.95	0.07	54,54,54,54	0
57	MG	1a	1797	1/1	0.95	0.14	56,56,56,56	0
57	MG	1a	1798	1/1	0.95	0.09	42,42,42,42	0
57	MG	2A	3113	1/1	0.95	0.09	45,45,45,45	0
57	MG	2a	1802	1/1	0.95	0.11	74,74,74,74	0
57	MG	1a	1799	1/1	0.95	0.14	79,79,79,79	0
57	MG	2A	3452	1/1	0.95	0.15	22,22,22,22	0
57	MG	1A	3158	1/1	0.95	0.16	42,42,42,42	0
57	MG	2A	3454	1/1	0.95	0.09	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3588	1/1	0.95	0.15	37,37,37,37	0
57	MG	1E	310	1/1	0.95	0.56	38,38,38,38	0
57	MG	2A	3457	1/1	0.95	0.59	66,66,66,66	0
57	MG	2T	3500	1/1	0.95	0.12	58,58,58,58	0
57	MG	1a	1803	1/1	0.95	0.10	66,66,66,66	0
57	MG	1A	3450	1/1	0.95	0.29	47,47,47,47	0
57	MG	2U	201	1/1	0.95	0.78	59,59,59,59	0
57	MG	2U	202	1/1	0.95	0.47	51,51,51,51	0
57	MG	2V	202	1/1	0.95	0.55	45,45,45,45	0
57	MG	2A	3684	1/1	0.95	0.11	59,59,59,59	0
57	MG	2A	3460	1/1	0.95	0.21	67,67,67,67	0
57	MG	1A	3232	1/1	0.95	0.12	43,43,43,43	0
57	MG	1A	3452	1/1	0.95	0.12	30,30,30,30	0
57	MG	2A	3463	1/1	0.95	0.41	62,62,62,62	0
57	MG	2Y	201	1/1	0.95	0.24	61,61,61,61	0
57	MG	2A	3690	1/1	0.95	0.11	62,62,62,62	0
57	MG	2A	3464	1/1	0.95	0.30	56,56,56,56	0
57	MG	2A	3692	1/1	0.95	0.12	64,64,64,64	0
57	MG	2A	3693	1/1	0.95	0.09	77,77,77,77	0
57	MG	1A	3512	1/1	0.95	0.17	40,40,40,40	0
57	MG	1A	3905	1/1	0.95	0.14	35,35,35,35	0
57	MG	1A	3594	1/1	0.95	0.14	31,31,31,31	0
57	MG	23	103	1/1	0.95	0.11	57,57,57,57	0
57	MG	1a	1813	1/1	0.95	0.14	61,61,61,61	0
57	MG	1A	3686	1/1	0.95	0.18	17,17,17,17	0
57	MG	2A	3472	1/1	0.95	0.14	69,69,69,69	0
57	MG	1A	3233	1/1	0.95	0.10	60,60,60,60	0
57	MG	1F	306	1/1	0.95	0.12	36,36,36,36	0
57	MG	1a	1818	1/1	0.95	0.18	53,53,53,53	0
57	MG	1A	3597	1/1	0.95	0.22	29,29,29,29	0
57	MG	2A	3477	1/1	0.95	0.27	41,41,41,41	0
57	MG	1F	311	1/1	0.95	0.19	40,40,40,40	0
57	MG	1a	1821	1/1	0.95	0.24	65,65,65,65	0
57	MG	1A	3454	1/1	0.95	0.28	28,28,28,28	0
57	MG	1A	3690	1/1	0.95	0.18	18,18,18,18	0
57	MG	1A	4032	1/1	0.95	0.26	52,52,52,52	0
57	MG	1A	3455	1/1	0.95	0.22	30,30,30,30	0
57	MG	1G	204	1/1	0.95	0.19	50,50,50,50	0
57	MG	1A	3408	1/1	0.95	0.41	45,45,45,45	0
57	MG	1A	3194	1/1	0.95	0.27	29,29,29,29	0
57	MG	2A	3716	1/1	0.95	0.10	33,33,33,33	0
57	MG	1a	1658	1/1	0.95	0.14	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3919	1/1	0.95	0.12	34,34,34,34	0
57	MG	2A	3490	1/1	0.95	0.22	47,47,47,47	0
59	ZN	1n	103	1/1	0.95	0.17	66,66,66,66	0
57	MG	1m	3002	1/1	0.95	0.29	56,56,56,56	0
57	MG	2A	3493	1/1	0.95	0.25	57,57,57,57	0
57	MG	2A	3722	1/1	0.95	0.08	50,50,50,50	0
57	MG	1A	3810	1/1	0.95	0.12	44,44,44,44	0
57	MG	1A	3923	1/1	0.96	0.18	36,36,36,36	0
57	MG	1a	1753	1/1	0.96	0.22	30,30,30,30	0
57	MG	1A	3067	1/1	0.96	0.19	28,28,28,28	0
57	MG	1a	1609	1/1	0.96	0.25	53,53,53,53	0
57	MG	2A	3555	1/1	0.96	0.23	58,58,58,58	0
57	MG	2A	3762	1/1	0.96	0.16	35,35,35,35	0
57	MG	1A	3318	1/1	0.96	0.29	41,41,41,41	0
57	MG	1A	3740	1/1	0.96	0.19	20,20,20,20	0
57	MG	2A	3060	1/1	0.96	0.17	58,58,58,58	0
57	MG	1A	3593	1/1	0.96	0.17	23,23,23,23	0
57	MG	1E	308	1/1	0.96	0.26	48,48,48,48	0
57	MG	1A	3355	1/1	0.96	0.29	27,27,27,27	0
57	MG	1A	3836	1/1	0.96	0.08	41,41,41,41	0
57	MG	2A	3220	1/1	0.96	0.30	49,49,49,49	0
57	MG	2A	3771	1/1	0.96	0.05	51,51,51,51	0
57	MG	2A	3564	1/1	0.96	0.17	58,58,58,58	0
57	MG	2A	3774	1/1	0.96	0.09	47,47,47,47	0
57	MG	1A	3930	1/1	0.96	0.14	28,28,28,28	0
57	MG	1a	1619	1/1	0.96	0.14	52,52,52,52	0
57	MG	2A	3777	1/1	0.96	0.08	37,37,37,37	0
57	MG	1A	3662	1/1	0.96	0.19	31,31,31,31	0
57	MG	1A	3663	1/1	0.96	0.17	26,26,26,26	0
57	MG	2A	3569	1/1	0.96	0.17	51,51,51,51	0
57	MG	1A	3745	1/1	0.96	0.18	66,66,66,66	0
57	MG	1a	1624	1/1	0.96	0.12	50,50,50,50	0
57	MG	2A	3227	1/1	0.96	0.51	42,42,42,42	0
57	MG	1A	3536	1/1	0.96	0.12	30,30,30,30	0
57	MG	1A	3357	1/1	0.96	0.12	57,57,57,57	0
57	MG	2A	3388	1/1	0.96	0.09	73,73,73,73	0
57	MG	1F	301	1/1	0.96	0.38	38,38,38,38	0
57	MG	1A	3278	1/1	0.96	0.40	37,37,37,37	0
57	MG	1A	3846	1/1	0.96	0.30	41,41,41,41	0
57	MG	1a	1776	1/1	0.96	0.06	43,43,43,43	0
57	MG	1A	3280	1/1	0.96	0.24	30,30,30,30	0
57	MG	1A	3600	1/1	0.96	0.42	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3669	1/1	0.96	0.08	36,36,36,36	0
57	MG	1F	312	1/1	0.96	0.27	28,28,28,28	0
57	MG	2a	1670	1/1	0.96	0.10	49,49,49,49	0
57	MG	2A	3798	1/1	0.96	0.08	58,58,58,58	0
57	MG	1A	3850	1/1	0.96	0.11	36,36,36,36	0
57	MG	2A	3587	1/1	0.96	0.18	65,65,65,65	0
57	MG	1A	3360	1/1	0.96	0.21	61,61,61,61	0
57	MG	2A	3802	1/1	0.96	0.15	52,52,52,52	0
57	MG	1A	3245	1/1	0.96	0.24	46,46,46,46	0
57	MG	2A	3805	1/1	0.96	0.13	36,36,36,36	0
57	MG	1A	3757	1/1	0.96	0.13	55,55,55,55	0
57	MG	1a	1785	1/1	0.96	0.13	46,46,46,46	0
57	MG	1A	3947	1/1	0.96	0.14	51,51,51,51	0
57	MG	1A	3092	1/1	0.96	0.16	21,21,21,21	0
57	MG	1a	1788	1/1	0.96	0.18	65,65,65,65	0
57	MG	2A	3596	1/1	0.96	0.17	66,66,66,66	0
57	MG	1A	4051	1/1	0.96	0.24	31,31,31,31	0
57	MG	1a	1790	1/1	0.96	0.09	49,49,49,49	0
57	MG	1a	1792	1/1	0.96	0.11	55,55,55,55	0
57	MG	1A	3543	1/1	0.96	0.28	36,36,36,36	0
57	MG	1A	3544	1/1	0.96	0.30	47,47,47,47	0
57	MG	1a	1795	1/1	0.96	0.09	62,62,62,62	0
57	MG	2A	3819	1/1	0.96	0.23	54,54,54,54	0
57	MG	1N	205	1/1	0.96	0.28	43,43,43,43	0
57	MG	1A	3113	1/1	0.96	0.10	31,31,31,31	0
57	MG	1A	3677	1/1	0.96	0.15	34,34,34,34	0
57	MG	2a	1699	1/1	0.96	0.12	57,57,57,57	0
57	MG	1A	3956	1/1	0.96	0.05	53,53,53,53	0
57	MG	1A	3766	1/1	0.96	0.13	36,36,36,36	0
57	MG	1A	4058	1/1	0.96	0.21	18,18,18,18	0
57	MG	2A	3828	1/1	0.96	0.10	29,29,29,29	0
57	MG	2A	3259	1/1	0.96	0.38	54,54,54,54	0
57	MG	1A	3607	1/1	0.96	0.44	51,51,51,51	0
57	MG	2A	3831	1/1	0.96	0.09	57,57,57,57	0
57	MG	2A	3612	1/1	0.96	0.13	33,33,33,33	0
57	MG	1a	1650	1/1	0.96	0.07	54,54,54,54	0
57	MG	2A	3424	1/1	0.96	0.17	55,55,55,55	0
57	MG	1A	3406	1/1	0.96	0.54	34,34,34,34	0
57	MG	1a	1653	1/1	0.96	0.08	53,53,53,53	0
57	MG	2A	3427	1/1	0.96	0.08	69,69,69,69	0
57	MG	1A	3287	1/1	0.96	0.25	36,36,36,36	0
57	MG	2a	1715	1/1	0.96	0.13	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	4062	1/1	0.96	0.11	58,58,58,58	0
57	MG	2A	3266	1/1	0.96	0.46	69,69,69,69	0
57	MG	2A	3623	1/1	0.96	0.21	34,34,34,34	0
57	MG	1A	3115	1/1	0.96	0.40	39,39,39,39	0
57	MG	2A	3110	1/1	0.96	0.11	61,61,61,61	0
57	MG	1a	1812	1/1	0.96	0.14	67,67,67,67	0
57	MG	1Q	201	1/1	0.96	0.36	39,39,39,39	0
57	MG	2A	3114	1/1	0.96	0.08	66,66,66,66	0
57	MG	1A	3010	1/1	0.96	0.20	27,27,27,27	0
57	MG	2A	3273	1/1	0.96	0.14	56,56,56,56	0
57	MG	1a	1815	1/1	0.96	0.14	59,59,59,59	0
57	MG	2a	1727	1/1	0.96	0.20	69,69,69,69	0
57	MG	1A	3683	1/1	0.96	0.16	37,37,37,37	0
57	MG	1A	3081	1/1	0.96	0.20	36,36,36,36	0
57	MG	2a	1730	1/1	0.96	0.25	70,70,70,70	0
57	MG	2A	3442	1/1	0.96	0.27	37,37,37,37	0
57	MG	1Q	205	1/1	0.96	0.13	44,44,44,44	0
57	MG	2A	3641	1/1	0.96	0.07	51,51,51,51	0
57	MG	2a	1734	1/1	0.96	0.24	60,60,60,60	0
57	MG	1R	201	1/1	0.96	0.17	35,35,35,35	0
57	MG	1A	3613	1/1	0.96	0.24	46,46,46,46	0
57	MG	1A	3193	1/1	0.96	0.34	27,27,27,27	0
57	MG	2a	1738	1/1	0.96	0.07	55,55,55,55	0
57	MG	1A	3496	1/1	0.96	0.19	34,34,34,34	0
57	MG	1a	1823	1/1	0.96	0.14	62,62,62,62	0
57	MG	1A	3166	1/1	0.96	0.33	34,34,34,34	0
57	MG	2A	3648	1/1	0.96	0.11	64,64,64,64	0
57	MG	1b	302	1/1	0.96	0.16	77,77,77,77	0
57	MG	2A	3650	1/1	0.96	0.13	43,43,43,43	0
57	MG	2a	1745	1/1	0.96	0.11	64,64,64,64	0
57	MG	1a	1669	1/1	0.96	0.08	61,61,61,61	0
57	MG	2A	3652	1/1	0.96	0.07	63,63,63,63	0
57	MG	1A	3196	1/1	0.96	0.26	29,29,29,29	0
57	MG	1A	3224	1/1	0.96	0.26	34,34,34,34	0
57	MG	1A	4076	1/1	0.96	0.14	37,37,37,37	0
57	MG	1a	1673	1/1	0.96	0.10	59,59,59,59	0
57	MG	1A	3140	1/1	0.96	0.16	26,26,26,26	0
57	MG	2a	1754	1/1	0.96	0.21	41,41,41,41	0
57	MG	2a	1755	1/1	0.96	0.11	57,57,57,57	0
57	MG	1A	4078	1/1	0.96	0.17	52,52,52,52	0
57	MG	1A	3692	1/1	0.96	0.14	18,18,18,18	0
57	MG	1A	3373	1/1	0.96	0.18	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3198	1/1	0.96	0.18	41,41,41,41	0
57	MG	1A	3142	1/1	0.96	0.10	51,51,51,51	0
57	MG	1A	3009	1/1	0.96	0.17	24,24,24,24	0
57	MG	2B	218	1/1	0.96	0.13	76,76,76,76	0
57	MG	1A	3977	1/1	0.96	0.17	45,45,45,45	0
57	MG	1A	3564	1/1	0.96	0.40	33,33,33,33	0
57	MG	2A	3467	1/1	0.96	0.14	54,54,54,54	0
57	MG	2A	3468	1/1	0.96	0.42	52,52,52,52	0
57	MG	2A	3671	1/1	0.96	0.22	64,64,64,64	0
57	MG	1A	3979	1/1	0.96	0.21	39,39,39,39	0
57	MG	1A	3301	1/1	0.96	0.32	51,51,51,51	0
57	MG	1A	3884	1/1	0.96	0.17	41,41,41,41	0
57	MG	1w	107	1/1	0.96	0.21	64,64,64,64	0
57	MG	1A	3792	1/1	0.96	0.12	40,40,40,40	0
57	MG	2E	304	1/1	0.96	0.10	38,38,38,38	0
57	MG	2A	3148	1/1	0.96	0.17	73,73,73,73	0
57	MG	2E	306	1/1	0.96	0.16	31,31,31,31	0
57	MG	1A	3083	1/1	0.96	0.18	36,36,36,36	0
57	MG	1A	3703	1/1	0.96	0.14	26,26,26,26	0
57	MG	1A	3795	1/1	0.96	0.10	22,22,22,22	0
57	MG	1W	203	1/1	0.96	0.19	62,62,62,62	0
57	MG	1W	204	1/1	0.96	0.35	30,30,30,30	0
57	MG	1A	3303	1/1	0.96	0.43	33,33,33,33	0
57	MG	1A	3015	1/1	0.96	0.35	36,36,36,36	0
57	MG	1X	105	1/1	0.96	0.12	48,48,48,48	0
57	MG	1X	106	1/1	0.96	0.17	30,30,30,30	0
57	MG	1A	3513	1/1	0.96	0.12	52,52,52,52	0
57	MG	2A	3160	1/1	0.96	0.12	35,35,35,35	0
57	MG	1A	3342	1/1	0.96	0.14	58,58,58,58	0
57	MG	1Z	302	1/1	0.96	0.25	51,51,51,51	0
57	MG	1A	3991	1/1	0.96	0.24	20,20,20,20	0
57	MG	1A	3710	1/1	0.96	0.15	27,27,27,27	0
57	MG	10	104	1/1	0.96	0.44	32,32,32,32	0
57	MG	1A	3573	1/1	0.96	0.17	15,15,15,15	0
57	MG	1A	3574	1/1	0.96	0.20	45,45,45,45	0
57	MG	1B	208	1/1	0.96	0.19	65,65,65,65	0
57	MG	1a	1710	1/1	0.96	0.27	60,60,60,60	0
57	MG	2A	3010	1/1	0.96	0.09	58,58,58,58	0
57	MG	2A	3498	1/1	0.96	0.16	63,63,63,63	0
57	MG	2V	201	1/1	0.96	0.10	66,66,66,66	0
57	MG	1A	3122	1/1	0.96	0.32	39,39,39,39	0
57	MG	2a	1804	1/1	0.96	0.19	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3997	1/1	0.96	0.07	39,39,39,39	0
57	MG	2A	3704	1/1	0.96	0.13	34,34,34,34	0
57	MG	1A	3714	1/1	0.96	0.15	33,33,33,33	0
57	MG	1A	3205	1/1	0.96	0.19	21,21,21,21	0
57	MG	12	101	1/1	0.96	0.20	39,39,39,39	0
57	MG	13	101	1/1	0.96	0.13	32,32,32,32	0
57	MG	1B	213	1/1	0.96	0.19	30,30,30,30	0
57	MG	1A	3903	1/1	0.96	0.09	37,37,37,37	0
57	MG	1B	216	1/1	0.96	0.15	59,59,59,59	0
57	MG	1B	217	1/1	0.96	0.16	46,46,46,46	0
57	MG	2A	3510	1/1	0.96	0.16	39,39,39,39	0
57	MG	1B	218	1/1	0.96	0.09	51,51,51,51	0
57	MG	2A	3026	1/1	0.96	0.22	48,48,48,48	0
57	MG	1A	3716	1/1	0.96	0.17	36,36,36,36	0
57	MG	1A	3309	1/1	0.96	0.28	53,53,53,53	0
57	MG	1A	3906	1/1	0.96	0.19	23,23,23,23	0
57	MG	1A	3100	1/1	0.96	0.15	38,38,38,38	0
57	MG	25	105	1/1	0.96	0.38	58,58,58,58	0
57	MG	1A	3908	1/1	0.96	0.18	22,22,22,22	0
57	MG	2A	3519	1/1	0.96	0.10	54,54,54,54	0
57	MG	27	102	1/1	0.96	0.40	47,47,47,47	0
57	MG	2A	3344	1/1	0.96	0.10	66,66,66,66	0
57	MG	2f	201	1/1	0.96	0.10	45,45,45,45	0
57	MG	2A	3723	1/1	0.96	0.14	64,64,64,64	0
57	MG	1A	3430	1/1	0.96	0.24	49,49,49,49	0
57	MG	2A	3523	1/1	0.96	0.44	67,67,67,67	0
57	MG	2A	3346	1/1	0.96	0.17	58,58,58,58	0
57	MG	1A	3347	1/1	0.96	0.25	43,43,43,43	0
57	MG	17	101	1/1	0.96	0.16	34,34,34,34	0
57	MG	2A	3528	1/1	0.96	0.18	37,37,37,37	0
57	MG	1A	3646	1/1	0.96	0.13	47,47,47,47	0
57	MG	2A	3038	1/1	0.96	0.14	26,26,26,26	0
57	MG	1a	1732	1/1	0.96	0.25	63,63,63,63	0
57	MG	2t	201	1/1	0.96	0.13	48,48,48,48	0
57	MG	1A	3086	1/1	0.96	0.29	28,28,28,28	0
57	MG	1A	3045	1/1	0.96	0.21	34,34,34,34	0
57	MG	18	103	1/1	0.96	0.14	38,38,38,38	0
57	MG	2A	3535	1/1	0.96	0.11	50,50,50,50	0
57	MG	1A	3476	1/1	0.96	0.13	46,46,46,46	0
57	MG	1A	3020	1/1	0.96	0.13	34,34,34,34	0
57	MG	2A	3744	1/1	0.96	0.18	59,59,59,59	0
57	MG	1A	3527	1/1	0.96	0.16	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3918	1/1	0.96	0.23	43,43,43,43	0
57	MG	1A	3064	1/1	0.96	0.26	31,31,31,31	0
57	MG	1A	3039	1/1	0.96	0.48	31,31,31,31	0
57	MG	2A	3544	1/1	0.96	0.13	51,51,51,51	0
57	MG	1A	3735	1/1	0.96	0.12	35,35,35,35	0
57	MG	2a	1622	1/1	0.96	0.14	58,58,58,58	0
57	MG	2a	1623	1/1	0.96	0.10	65,65,65,65	0
57	MG	2A	3547	1/1	0.96	0.22	40,40,40,40	0
57	MG	1D	305	1/1	0.96	0.31	41,41,41,41	0
57	MG	2A	3753	1/1	0.96	0.14	51,51,51,51	0
59	ZN	25	106	1/1	0.96	0.23	60,60,60,60	0
57	MG	1A	3532	1/1	0.96	0.26	60,60,60,60	0
57	MG	1D	308	1/1	0.96	0.18	45,45,45,45	0
57	MG	2A	3112	1/1	0.97	0.10	49,49,49,49	0
57	MG	1A	3066	1/1	0.97	0.24	31,31,31,31	0
57	MG	1E	303	1/1	0.97	0.21	27,27,27,27	0
57	MG	2a	1691	1/1	0.97	0.17	42,42,42,42	0
57	MG	2A	3537	1/1	0.97	0.11	50,50,50,50	0
57	MG	2A	3697	1/1	0.97	0.14	60,60,60,60	0
57	MG	1E	304	1/1	0.97	0.23	27,27,27,27	0
57	MG	1A	3694	1/1	0.97	0.12	20,20,20,20	0
57	MG	16	101	1/1	0.97	0.31	41,41,41,41	0
57	MG	1A	3778	1/1	0.97	0.18	42,42,42,42	0
57	MG	2A	3119	1/1	0.97	0.24	65,65,65,65	0
57	MG	1A	3695	1/1	0.97	0.16	18,18,18,18	0
57	MG	1A	3696	1/1	0.97	0.21	27,27,27,27	0
57	MG	17	102	1/1	0.97	0.15	26,26,26,26	0
57	MG	17	103	1/1	0.97	0.26	29,29,29,29	0
57	MG	1A	3160	1/1	0.97	0.21	25,25,25,25	0
57	MG	1A	3393	1/1	0.97	0.22	45,45,45,45	0
57	MG	1A	3562	1/1	0.97	0.18	48,48,48,48	0
57	MG	2a	1706	1/1	0.97	0.09	69,69,69,69	0
57	MG	1A	3105	1/1	0.97	0.15	29,29,29,29	0
57	MG	1A	3011	1/1	0.97	0.16	39,39,39,39	0
57	MG	1A	3449	1/1	0.97	0.28	41,41,41,41	0
57	MG	1A	3504	1/1	0.97	0.25	25,25,25,25	0
57	MG	1A	3053	1/1	0.97	0.14	48,48,48,48	0
57	MG	1A	3506	1/1	0.97	0.29	39,39,39,39	0
57	MG	1A	3003	1/1	0.97	0.18	23,23,23,23	0
57	MG	1F	307	1/1	0.97	0.15	36,36,36,36	0
57	MG	1F	309	1/1	0.97	0.15	23,23,23,23	0
57	MG	1x	109	1/1	0.97	0.11	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3249	1/1	0.97	0.40	33,33,33,33	0
57	MG	1A	3509	1/1	0.97	0.24	71,71,71,71	0
57	MG	1A	3109	1/1	0.97	0.30	31,31,31,31	0
57	MG	1A	3641	1/1	0.97	0.18	20,20,20,20	0
57	MG	2A	3724	1/1	0.97	0.11	57,57,57,57	0
57	MG	1A	3796	1/1	0.97	0.16	22,22,22,22	0
57	MG	2A	3417	1/1	0.97	0.25	59,59,59,59	0
57	MG	1A	3642	1/1	0.97	0.16	42,42,42,42	0
57	MG	2E	309	1/1	0.97	0.23	58,58,58,58	0
57	MG	1a	1731	1/1	0.97	0.12	49,49,49,49	0
57	MG	2A	3570	1/1	0.97	0.10	40,40,40,40	0
57	MG	2A	3731	1/1	0.97	0.24	52,52,52,52	0
57	MG	2A	3571	1/1	0.97	0.17	31,31,31,31	0
57	MG	2F	305	1/1	0.97	0.38	40,40,40,40	0
57	MG	1A	3300	1/1	0.97	0.14	32,32,32,32	0
57	MG	1A	3251	1/1	0.97	0.25	37,37,37,37	0
57	MG	2A	3736	1/1	0.97	0.29	40,40,40,40	0
57	MG	1a	1735	1/1	0.97	0.35	47,47,47,47	0
57	MG	1a	1736	1/1	0.97	0.08	67,67,67,67	0
57	MG	1a	1614	1/1	0.97	0.25	60,60,60,60	0
57	MG	1a	1739	1/1	0.97	0.21	58,58,58,58	0
57	MG	1A	3889	1/1	0.97	0.21	35,35,35,35	0
57	MG	2A	3152	1/1	0.97	0.45	38,38,38,38	0
57	MG	1A	3645	1/1	0.97	0.21	15,15,15,15	0
57	MG	2A	3290	1/1	0.97	0.19	56,56,56,56	0
57	MG	1A	3168	1/1	0.97	0.22	31,31,31,31	0
57	MG	1A	3071	1/1	0.97	0.28	22,22,22,22	0
57	MG	1N	204	1/1	0.97	0.20	37,37,37,37	0
57	MG	2A	3021	1/1	0.97	0.11	24,24,24,24	0
57	MG	1A	3805	1/1	0.97	0.09	38,38,38,38	0
57	MG	1a	1621	1/1	0.97	0.11	41,41,41,41	0
57	MG	1A	3720	1/1	0.97	0.15	20,20,20,20	0
57	MG	1A	3721	1/1	0.97	0.14	14,14,14,14	0
57	MG	1A	3136	1/1	0.97	0.19	26,26,26,26	0
57	MG	2A	3027	1/1	0.97	0.13	42,42,42,42	0
57	MG	2A	3028	1/1	0.97	0.40	51,51,51,51	0
57	MG	2a	1753	1/1	0.97	0.11	50,50,50,50	0
57	MG	1A	3723	1/1	0.97	0.18	28,28,28,28	0
57	MG	1A	3138	1/1	0.97	0.34	42,42,42,42	0
57	MG	1A	3111	1/1	0.97	0.15	35,35,35,35	0
57	MG	1A	3356	1/1	0.97	0.16	36,36,36,36	0
57	MG	1A	3308	1/1	0.97	0.27	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	4084	1/1	0.97	0.07	41,41,41,41	0
57	MG	1A	3257	1/1	0.97	0.10	72,72,72,72	0
57	MG	1A	4086	1/1	0.97	0.23	63,63,63,63	0
57	MG	1A	3112	1/1	0.97	0.18	27,27,27,27	0
57	MG	1A	3993	1/1	0.97	0.24	39,39,39,39	0
57	MG	1A	3311	1/1	0.97	0.17	26,26,26,26	0
57	MG	1A	3014	1/1	0.97	0.15	28,28,28,28	0
57	MG	1a	1764	1/1	0.97	0.12	61,61,61,61	0
57	MG	1A	3658	1/1	0.97	0.18	16,16,16,16	0
57	MG	1A	3823	1/1	0.97	0.10	42,42,42,42	0
57	MG	1R	203	1/1	0.97	0.18	37,37,37,37	0
57	MG	2A	3773	1/1	0.97	0.10	51,51,51,51	0
57	MG	1A	3260	1/1	0.97	0.16	34,34,34,34	0
57	MG	1A	3912	1/1	0.97	0.08	37,37,37,37	0
57	MG	2a	1774	1/1	0.97	0.18	59,59,59,59	0
57	MG	1A	3176	1/1	0.97	0.11	25,25,25,25	0
57	MG	1A	3177	1/1	0.97	0.25	23,23,23,23	0
57	MG	2a	1777	1/1	0.97	0.10	66,66,66,66	0
57	MG	2A	3049	1/1	0.97	0.12	28,28,28,28	0
57	MG	2A	3616	1/1	0.97	0.26	65,65,65,65	0
57	MG	1A	3529	1/1	0.97	0.20	70,70,70,70	0
57	MG	2A	3781	1/1	0.97	0.07	51,51,51,51	0
57	MG	1B	201	1/1	0.97	0.23	53,53,53,53	0
57	MG	1A	4004	1/1	0.97	0.20	17,17,17,17	0
57	MG	1a	1775	1/1	0.97	0.09	62,62,62,62	0
57	MG	1A	3057	1/1	0.97	0.20	22,22,22,22	0
57	MG	1A	3179	1/1	0.97	0.19	34,34,34,34	0
57	MG	1A	3028	1/1	0.97	0.28	29,29,29,29	0
57	MG	1A	3473	1/1	0.97	0.17	30,30,30,30	0
57	MG	2a	1789	1/1	0.97	0.17	65,65,65,65	0
57	MG	1A	3008	1/1	0.97	0.22	25,25,25,25	0
57	MG	1a	1652	1/1	0.97	0.14	66,66,66,66	0
57	MG	2A	3630	1/1	0.97	0.16	46,46,46,46	0
57	MG	1A	3146	1/1	0.97	0.16	29,29,29,29	0
57	MG	1A	3746	1/1	0.97	0.12	46,46,46,46	0
57	MG	1A	3077	1/1	0.97	0.13	32,32,32,32	0
57	MG	1A	3030	1/1	0.97	0.28	28,28,28,28	0
57	MG	2A	3797	1/1	0.97	0.10	62,62,62,62	0
57	MG	1A	4016	1/1	0.97	0.10	41,41,41,41	0
57	MG	1B	214	1/1	0.97	0.30	62,62,62,62	0
57	MG	1A	3838	1/1	0.97	0.16	24,24,24,24	0
57	MG	1A	3149	1/1	0.97	0.38	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3426	1/1	0.97	0.21	56,56,56,56	0
57	MG	2A	3803	1/1	0.97	0.10	39,39,39,39	0
57	MG	1a	1791	1/1	0.97	0.21	52,52,52,52	0
57	MG	2A	3486	1/1	0.97	0.17	53,53,53,53	0
57	MG	1W	201	1/1	0.97	0.11	36,36,36,36	0
57	MG	1A	3324	1/1	0.97	0.22	25,25,25,25	0
57	MG	1A	3150	1/1	0.97	0.41	40,40,40,40	0
57	MG	2a	1810	1/1	0.97	0.04	73,73,73,73	0
57	MG	2a	1631	1/1	0.97	0.19	59,59,59,59	0
57	MG	1A	3844	1/1	0.97	0.12	51,51,51,51	0
57	MG	1a	1796	1/1	0.97	0.10	66,66,66,66	0
57	MG	2A	3492	1/1	0.97	0.29	56,56,56,56	0
57	MG	1a	1667	1/1	0.97	0.17	68,68,68,68	0
57	MG	1W	206	1/1	0.97	0.13	37,37,37,37	0
57	MG	1A	4023	1/1	0.97	0.08	61,61,61,61	0
57	MG	2A	3653	1/1	0.97	0.10	65,65,65,65	0
57	MG	1X	101	1/1	0.97	0.34	32,32,32,32	0
57	MG	1A	3274	1/1	0.97	0.28	33,33,33,33	0
57	MG	1X	103	1/1	0.97	0.34	46,46,46,46	0
57	MG	1A	3096	1/1	0.97	0.09	30,30,30,30	0
57	MG	2A	3821	1/1	0.97	0.13	61,61,61,61	0
57	MG	2a	1824	1/1	0.97	0.24	61,61,61,61	0
57	MG	1A	3933	1/1	0.97	0.33	35,35,35,35	0
57	MG	1A	3276	1/1	0.97	0.41	38,38,38,38	0
57	MG	1Y	202	1/1	0.97	0.65	46,46,46,46	0
57	MG	2A	3825	1/1	0.97	0.11	37,37,37,37	0
57	MG	1a	1808	1/1	0.97	0.09	46,46,46,46	0
57	MG	1A	3031	1/1	0.97	0.16	28,28,28,28	0
57	MG	2A	3663	1/1	0.97	0.14	39,39,39,39	0
57	MG	1A	3032	1/1	0.97	0.17	24,24,24,24	0
57	MG	1A	3279	1/1	0.97	0.17	21,21,21,21	0
57	MG	10	102	1/1	0.97	0.17	41,41,41,41	0
57	MG	2A	3508	1/1	0.97	0.09	26,26,26,26	0
57	MG	2A	3668	1/1	0.97	0.36	41,41,41,41	0
57	MG	1A	3190	1/1	0.97	0.23	29,29,29,29	0
57	MG	1A	3764	1/1	0.97	0.16	57,57,57,57	0
57	MG	2A	3365	1/1	0.97	0.18	39,39,39,39	0
57	MG	1A	3191	1/1	0.97	0.33	38,38,38,38	0
57	MG	1A	3192	1/1	0.97	0.14	41,41,41,41	0
57	MG	2a	1661	1/1	0.97	0.06	58,58,58,58	0
57	MG	2A	3368	1/1	0.97	0.13	56,56,56,56	0
57	MG	1A	3022	1/1	0.97	0.11	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3125	1/1	0.97	0.28	28,28,28,28	0
57	MG	1A	3337	1/1	0.97	0.13	53,53,53,53	0
57	MG	1a	1690	1/1	0.97	0.16	62,62,62,62	0
57	MG	2A	3845	1/1	0.97	0.22	41,41,41,41	0
57	MG	1D	301	1/1	0.97	0.17	29,29,29,29	0
57	MG	1D	302	1/1	0.97	0.52	43,43,43,43	0
57	MG	1A	4039	1/1	0.97	0.15	18,18,18,18	0
57	MG	1A	3195	1/1	0.97	0.25	26,26,26,26	0
57	MG	2A	3525	1/1	0.97	0.18	32,32,32,32	0
57	MG	1b	301	1/1	0.97	0.14	78,78,78,78	0
57	MG	1D	307	1/1	0.97	0.22	30,30,30,30	0
57	MG	1A	3771	1/1	0.97	0.18	18,18,18,18	0
57	MG	2A	3854	1/1	0.97	0.15	43,43,43,43	0
57	MG	1A	3621	1/1	0.97	0.17	21,21,21,21	0
57	MG	1a	1699	1/1	0.97	0.34	47,47,47,47	0
57	MG	1D	310	1/1	0.97	0.24	26,26,26,26	0
57	MG	1A	3016	1/1	0.97	0.34	58,58,58,58	0
59	ZN	29	501	1/1	0.97	0.13	71,71,71,71	0
57	MG	1A	3051	1/1	0.97	0.24	31,31,31,31	0
57	MG	1A	3856	1/1	0.98	0.17	33,33,33,33	0
57	MG	1A	3036	1/1	0.98	0.18	33,33,33,33	0
57	MG	1A	3858	1/1	0.98	0.13	33,33,33,33	0
57	MG	1B	235	1/1	0.98	0.09	44,44,44,44	0
57	MG	1a	1807	1/1	0.98	0.24	52,52,52,52	0
57	MG	1A	3987	1/1	0.98	0.11	42,42,42,42	0
57	MG	2A	3588	1/1	0.98	0.14	27,27,27,27	0
57	MG	1A	3117	1/1	0.98	0.29	25,25,25,25	0
57	MG	1A	3398	1/1	0.98	0.24	26,26,26,26	0
57	MG	1V	201	1/1	0.98	0.19	27,27,27,27	0
57	MG	1D	303	1/1	0.98	0.20	31,31,31,31	0
57	MG	1A	3800	1/1	0.98	0.19	22,22,22,22	0
57	MG	1A	3206	1/1	0.98	0.13	34,34,34,34	0
57	MG	1A	3802	1/1	0.98	0.17	43,43,43,43	0
57	MG	1A	3531	1/1	0.98	0.10	73,73,73,73	0
57	MG	1A	3055	1/1	0.98	0.24	30,30,30,30	0
57	MG	1A	3230	1/1	0.98	0.20	27,27,27,27	0
57	MG	1A	3231	1/1	0.98	0.46	29,29,29,29	0
57	MG	1D	312	1/1	0.98	0.16	30,30,30,30	0
57	MG	1A	3283	1/1	0.98	0.31	29,29,29,29	0
57	MG	1W	205	1/1	0.98	0.27	34,34,34,34	0
57	MG	1A	3284	1/1	0.98	0.44	31,31,31,31	0
57	MG	1A	3661	1/1	0.98	0.27	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3705	1/1	0.98	0.21	28,28,28,28	0
57	MG	1A	4073	1/1	0.98	0.20	23,23,23,23	0
57	MG	2a	1759	1/1	0.98	0.07	69,69,69,69	0
57	MG	1A	3872	1/1	0.98	0.25	20,20,20,20	0
57	MG	2A	3069	1/1	0.98	0.36	57,57,57,57	0
57	MG	2A	3173	1/1	0.98	0.15	37,37,37,37	0
57	MG	2A	3610	1/1	0.98	0.15	41,41,41,41	0
57	MG	1X	104	1/1	0.98	0.22	34,34,34,34	0
57	MG	1a	1734	1/1	0.98	0.35	47,47,47,47	0
57	MG	1A	4075	1/1	0.98	0.19	22,22,22,22	0
57	MG	2A	3735	1/1	0.98	0.08	59,59,59,59	0
57	MG	1A	4002	1/1	0.98	0.16	15,15,15,15	0
57	MG	1a	1737	1/1	0.98	0.16	61,61,61,61	0
57	MG	1A	3706	1/1	0.98	0.13	22,22,22,22	0
57	MG	1A	3813	1/1	0.98	0.24	15,15,15,15	0
57	MG	1A	4005	1/1	0.98	0.10	33,33,33,33	0
57	MG	1A	3758	1/1	0.98	0.15	41,41,41,41	0
57	MG	1A	3038	1/1	0.98	0.13	25,25,25,25	0
57	MG	2A	3394	1/1	0.98	0.07	64,64,64,64	0
57	MG	2A	3184	1/1	0.98	0.14	57,57,57,57	0
57	MG	1A	3939	1/1	0.98	0.21	56,56,56,56	0
57	MG	2A	3625	1/1	0.98	0.13	31,31,31,31	0
57	MG	1A	3578	1/1	0.98	0.31	31,31,31,31	0
57	MG	2A	3082	1/1	0.98	0.27	45,45,45,45	0
57	MG	2A	3628	1/1	0.98	0.15	35,35,35,35	0
57	MG	1w	102	1/1	0.98	0.05	57,57,57,57	0
57	MG	1A	3502	1/1	0.98	0.25	38,38,38,38	0
57	MG	2A	3631	1/1	0.98	0.12	39,39,39,39	0
57	MG	1F	303	1/1	0.98	0.51	32,32,32,32	0
57	MG	1A	3047	1/1	0.98	0.24	32,32,32,32	0
57	MG	2A	3403	1/1	0.98	0.31	50,50,50,50	0
57	MG	1a	1655	1/1	0.98	0.10	40,40,40,40	0
57	MG	1A	3005	1/1	0.98	0.18	32,32,32,32	0
57	MG	2A	3517	1/1	0.98	0.23	59,59,59,59	0
57	MG	1a	1750	1/1	0.98	0.17	47,47,47,47	0
57	MG	2A	3760	1/1	0.98	0.18	63,63,63,63	0
57	MG	2A	3639	1/1	0.98	0.15	35,35,35,35	0
57	MG	1A	3021	1/1	0.98	0.14	22,22,22,22	0
57	MG	1F	308	1/1	0.98	0.22	21,21,21,21	0
57	MG	1A	4014	1/1	0.98	0.16	16,16,16,16	0
57	MG	2a	1668	1/1	0.98	0.10	44,44,44,44	0
57	MG	1A	3822	1/1	0.98	0.17	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3070	1/1	0.98	0.20	14,14,14,14	0
57	MG	1A	3175	1/1	0.98	0.19	25,25,25,25	0
57	MG	1A	3948	1/1	0.98	0.19	12,12,12,12	0
57	MG	2a	1673	1/1	0.98	0.07	61,61,61,61	0
57	MG	1A	3626	1/1	0.98	0.19	20,20,20,20	0
57	MG	1A	3671	1/1	0.98	0.12	45,45,45,45	0
57	MG	2a	1676	1/1	0.98	0.13	71,71,71,71	0
57	MG	1A	3951	1/1	0.98	0.18	24,24,24,24	0
57	MG	2a	1678	1/1	0.98	0.08	67,67,67,67	0
57	MG	2a	1808	1/1	0.98	0.23	51,51,51,51	0
57	MG	1G	203	1/1	0.98	0.33	58,58,58,58	0
57	MG	1A	3262	1/1	0.98	0.16	48,48,48,48	0
57	MG	1A	3156	1/1	0.98	0.12	20,20,20,20	0
57	MG	15	103	1/1	0.98	0.43	22,22,22,22	0
57	MG	1A	3041	1/1	0.98	0.12	28,28,28,28	0
57	MG	2A	3422	1/1	0.98	0.11	51,51,51,51	0
57	MG	1A	3955	1/1	0.98	0.19	43,43,43,43	0
57	MG	15	106	1/1	0.98	0.26	37,37,37,37	0
57	MG	2a	1687	1/1	0.98	0.17	58,58,58,58	0
57	MG	1A	3890	1/1	0.98	0.14	32,32,32,32	0
57	MG	1A	3773	1/1	0.98	0.18	67,67,67,67	0
57	MG	2A	3007	1/1	0.98	0.14	48,48,48,48	0
57	MG	1A	3240	1/1	0.98	0.19	35,35,35,35	0
57	MG	2A	3009	1/1	0.98	0.15	42,42,42,42	0
57	MG	2A	3543	1/1	0.98	0.13	40,40,40,40	0
57	MG	1B	206	1/1	0.98	0.20	44,44,44,44	0
57	MG	1A	3217	1/1	0.98	0.21	38,38,38,38	0
57	MG	2A	3012	1/1	0.98	0.12	31,31,31,31	0
57	MG	2A	3013	1/1	0.98	0.14	40,40,40,40	0
57	MG	1A	3894	1/1	0.98	0.15	31,31,31,31	0
57	MG	1A	3242	1/1	0.98	0.44	30,30,30,30	0
57	MG	1A	3514	1/1	0.98	0.28	28,28,28,28	0
57	MG	2A	3017	1/1	0.98	0.13	51,51,51,51	0
57	MG	1A	3725	1/1	0.98	0.15	38,38,38,38	0
57	MG	2A	3795	1/1	0.98	0.09	66,66,66,66	0
57	MG	2A	3439	1/1	0.98	0.26	59,59,59,59	0
57	MG	2k	201	1/1	0.98	0.05	67,67,67,67	0
57	MG	1P	201	1/1	0.98	0.28	26,26,26,26	0
57	MG	1a	1684	1/1	0.98	0.21	48,48,48,48	0
57	MG	1a	1685	1/1	0.98	0.08	53,53,53,53	0
57	MG	1A	3268	1/1	0.98	0.23	36,36,36,36	0
57	MG	1A	3635	1/1	0.98	0.23	10,10,10,10	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2r	101	1/1	0.98	0.14	69,69,69,69	0
57	MG	1A	3839	1/1	0.98	0.13	28,28,28,28	0
57	MG	1A	3901	1/1	0.98	0.20	30,30,30,30	0
57	MG	1A	3141	1/1	0.98	0.23	15,15,15,15	0
57	MG	1A	3072	1/1	0.98	0.18	11,11,11,11	0
57	MG	1A	3001	1/1	0.98	0.12	36,36,36,36	0
57	MG	2A	3451	1/1	0.98	0.42	50,50,50,50	0
57	MG	2A	3808	1/1	0.98	0.15	42,42,42,42	0
57	MG	1A	3127	1/1	0.98	0.20	32,32,32,32	0
57	MG	1A	3390	1/1	0.98	0.20	22,22,22,22	0
57	MG	1Q	207	1/1	0.98	0.15	33,33,33,33	0
57	MG	1A	3733	1/1	0.98	0.12	12,12,12,12	0
57	MG	25	103	1/1	0.98	0.55	44,44,44,44	0
57	MG	1A	3043	1/1	0.98	0.45	30,30,30,30	0
57	MG	1A	3114	1/1	0.98	0.15	29,29,29,29	0
57	MG	1A	3023	1/1	0.98	0.18	13,13,13,13	0
57	MG	1A	3790	1/1	0.98	0.15	15,15,15,15	0
57	MG	1a	1611	1/1	0.98	0.18	21,21,21,21	0
57	MG	1A	3524	1/1	0.98	0.22	26,26,26,26	0
57	MG	1A	3561	1/1	0.98	0.14	23,23,23,23	0
57	MG	2A	3247	1/1	0.98	0.16	80,80,80,80	0
57	MG	1A	3739	1/1	0.98	0.18	38,38,38,38	0
57	MG	1A	3306	1/1	0.98	0.23	25,25,25,25	0
57	MG	1A	3395	1/1	0.98	0.34	40,40,40,40	0
57	MG	1A	3565	1/1	0.98	0.14	28,28,28,28	0
60	SF4	1d	501	8/8	0.98	0.16	60,70,77,81	0
60	SF4	2d	303	8/8	0.98	0.15	69,79,88,91	0
57	MG	1E	305	1/1	0.99	0.20	28,28,28,28	0
57	MG	1U	201	1/1	0.99	0.34	30,30,30,30	0
57	MG	1A	3097	1/1	0.99	0.20	15,15,15,15	0
57	MG	1E	307	1/1	0.99	0.10	26,26,26,26	0
57	MG	2A	3837	1/1	0.99	0.18	37,37,37,37	0
57	MG	1A	3201	1/1	0.99	0.23	22,22,22,22	0
57	MG	1A	3161	1/1	0.99	0.18	25,25,25,25	0
57	MG	2A	3617	1/1	0.99	0.09	37,37,37,37	0
57	MG	1A	3640	1/1	0.99	0.17	31,31,31,31	0
57	MG	1A	4072	1/1	0.99	0.19	11,11,11,11	0
57	MG	1A	3162	1/1	0.99	0.43	29,29,29,29	0
57	MG	1U	209	1/1	0.99	0.32	29,29,29,29	0
57	MG	1a	1760	1/1	0.99	0.14	44,44,44,44	0
57	MG	1A	3821	1/1	0.99	0.16	21,21,21,21	0
57	MG	1A	3563	1/1	0.99	0.16	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3213	1/1	0.99	0.20	27,27,27,27	0
57	MG	2E	308	1/1	0.99	0.17	32,32,32,32	0
57	MG	1A	3137	1/1	0.99	0.27	32,32,32,32	0
57	MG	1A	3825	1/1	0.99	0.22	22,22,22,22	0
57	MG	1A	3717	1/1	0.99	0.26	27,27,27,27	0
57	MG	1P	204	1/1	0.99	0.25	29,29,29,29	0
57	MG	1A	3596	1/1	0.99	0.22	24,24,24,24	0
57	MG	2A	3546	1/1	0.99	0.17	29,29,29,29	0
57	MG	2A	3144	1/1	0.99	0.15	26,26,26,26	0
57	MG	1F	304	1/1	0.99	0.16	27,27,27,27	0
57	MG	1A	4028	1/1	0.99	0.17	57,57,57,57	0
57	MG	1A	3292	1/1	0.99	0.16	53,53,53,53	0
57	MG	1D	304	1/1	0.99	0.19	17,17,17,17	0
57	MG	1A	3582	1/1	0.99	0.25	36,36,36,36	0
57	MG	1A	3013	1/1	0.99	0.15	24,24,24,24	0
57	MG	2A	3726	1/1	0.99	0.06	74,74,74,74	0
57	MG	1a	1698	1/1	0.99	0.29	49,49,49,49	0
57	MG	1Q	206	1/1	0.99	0.31	39,39,39,39	0
57	MG	1A	3037	1/1	0.99	0.23	21,21,21,21	0
57	MG	1A	3807	1/1	0.99	0.18	16,16,16,16	0
57	MG	2a	1663	1/1	0.99	0.18	56,56,56,56	0
57	MG	1A	3763	1/1	0.99	0.22	54,54,54,54	0
57	MG	2A	3687	1/1	0.99	0.15	34,34,34,34	0
59	ZN	1Y	203	1/1	0.99	0.15	57,57,57,57	0
57	MG	1A	3650	1/1	0.99	0.14	28,28,28,28	0
59	ZN	15	108	1/1	0.99	0.23	41,41,41,41	0
59	ZN	16	104	1/1	0.99	0.24	48,48,48,48	0
57	MG	1F	314	1/1	0.99	0.14	42,42,42,42	0
57	MG	1A	3282	1/1	0.99	0.19	31,31,31,31	0
57	MG	1A	3104	1/1	0.99	0.14	46,46,46,46	0
57	MG	2A	3521	1/1	0.99	0.10	40,40,40,40	0
57	MG	18	102	1/1	0.99	0.18	36,36,36,36	0
57	MG	1A	3084	1/1	0.99	0.15	25,25,25,25	0
57	MG	1A	3229	1/1	0.99	0.20	27,27,27,27	0
57	MG	1A	3747	1/1	0.99	0.09	47,47,47,47	0
57	MG	1A	3748	1/1	0.99	0.17	18,18,18,18	0
59	ZN	19	102	1/1	1.00	0.21	40,40,40,40	0

6.5 Other polymers ⓘ

There are no such residues in this entry.