



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 16, 2020 – 01:05 AM EST

PDB ID : 6XHW
Title : Crystal structure of the A2058-unmethylated *Thermus thermophilus* 70S ribosome in complex with mRNA, aminoacylated A- and P-site tRNAs, and deacylated E-site tRNA at 2.50Å resolution
Authors : Svetlov, M.S.; Syroegin, E.A.; Aleksandrova, E.V.; Atkinson, G.C.; Gregory, S.T.; Mankin, A.S.; Polikanov, Y.S.
Deposited on : 2020-06-19
Resolution : 2.50 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 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	:	2.15.1
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)	:	2.15.1

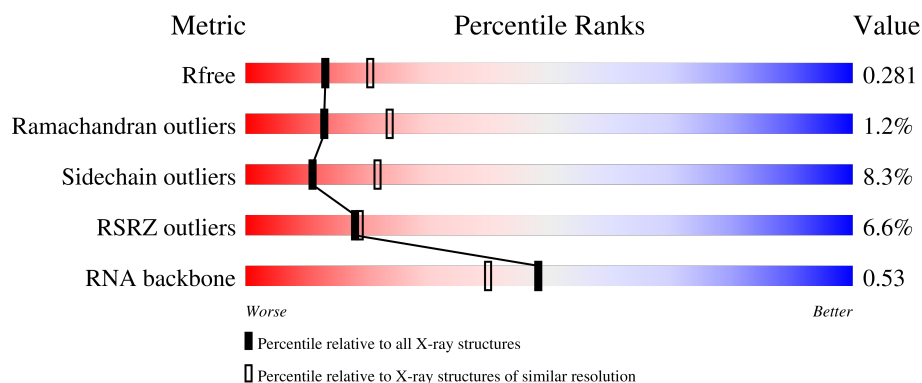
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)
RNA backbone	3102	1008 (2.84-2.16)

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>4%</div> <div>81%</div> <div>17%</div> <div>..</div> </div>
1	2A	2915	<div> <div>4%</div> <div>79%</div> <div>17%</div> <div>.</div> </div>
2	1B	121	<div> <div>90%</div> <div>9%</div> <div>.</div> </div>
2	2B	121	<div> <div>80%</div> <div>19%</div> <div>.</div> </div>
3	1D	276	<div> <div>%</div> <div>93%</div> <div>6%</div> </div>

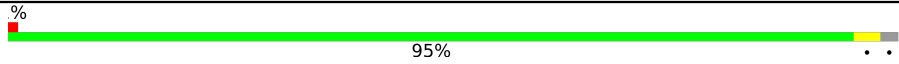
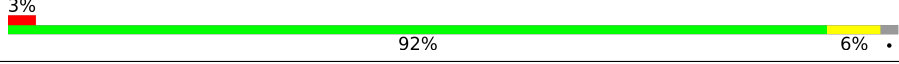
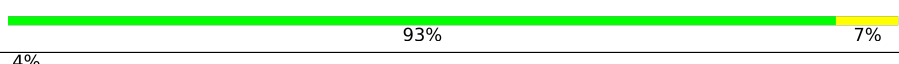

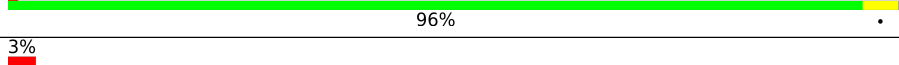
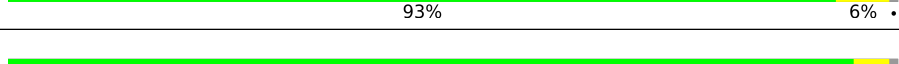
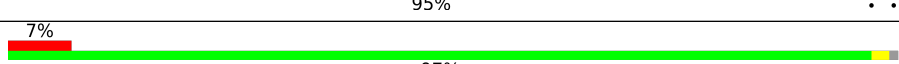
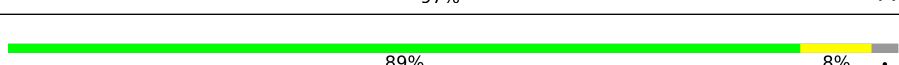
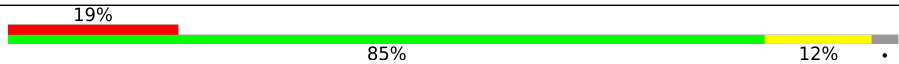


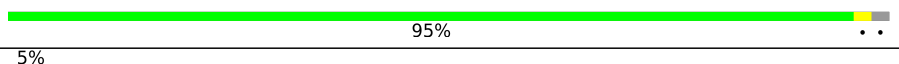
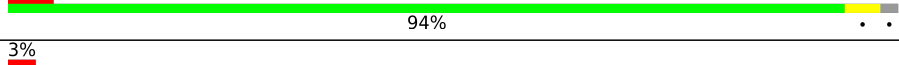
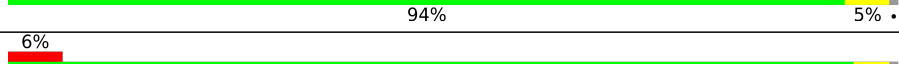
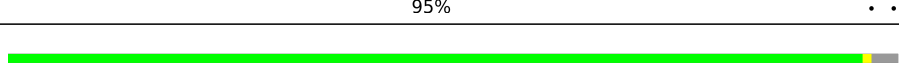
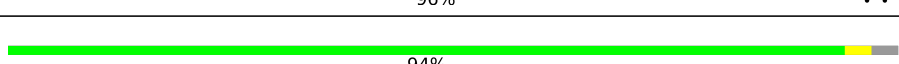
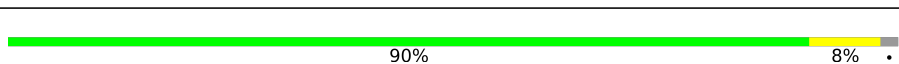
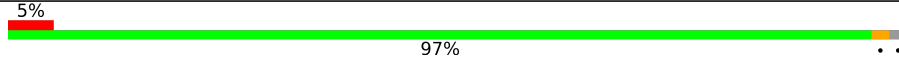


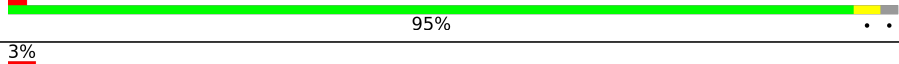
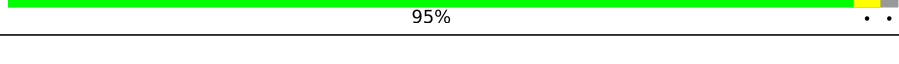



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Mol	Chain	Length	Quality of chain
3	2D	276	
4	1E	206	
4	2E	206	
5	1F	210	
5	2F	210	
6	1G	182	
6	2G	182	
7	1H	180	
7	2H	180	
8	1I	148	
8	2I	148	
9	1N	140	
9	2N	140	
10	1O	122	
10	2O	122	
11	1P	150	
11	2P	150	
12	1Q	141	
12	2Q	141	
13	1R	118	
13	2R	118	
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	
16	2U	118	
17	1V	101	
17	2V	101	
18	1W	113	
18	2W	113	
19	1X	96	
19	2X	96	
20	1Y	110	
20	2Y	110	
21	1Z	206	
21	2Z	206	
22	10	85	
22	20	85	
23	11	98	
23	21	98	
24	12	72	
24	22	72	
25	13	60	
25	23	60	
26	14	71	
26	24	71	
27	15	60	
27	25	60	
28	16	54	

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

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Mol	Chain	Length	Quality of chain
41	1j	105	
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	76	
54	2w	76	
55	1x	77	
55	2x	77	
56	1y	76	
56	2y	76	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	PSU	1y	55	-	-	-	X
56	PSU	2y	32	-	-	-	X
56	MIA	2y	37	-	-	-	X
56	PSU	2y	39	-	-	-	X
56	5MU	2y	54	-	-	-	X
56	PSU	2y	55	-	-	-	X
57	MG	1A	4274	-	-	-	X
57	MG	2A	3341	-	-	-	X
57	MG	2A	3482	-	-	-	X
57	MG	2A	3840	-	-	-	X
57	MG	2A	3917	-	-	-	X
57	MG	2A	3953	-	-	-	X
57	MG	2a	3002	-	-	-	X
57	MG	2a	3027	-	-	-	X
57	MG	2a	3030	-	-	-	X
57	MG	2a	3031	-	-	-	X
57	MG	2a	3050	-	-	-	X
57	MG	2a	3186	-	-	-	X

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 300196 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	2O	122	Total	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 mRNA.

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	1x	76	Total	C	N	O	P	S	0	0
			1635	731	296	530	76	2		
55	2x	76	Total	C	N	O	P	S	0	0
			1635	731	296	530	76	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1x	76	31H	-	expression tag	GB 1848949880
2x	76	31H	-	expression tag	GB 1848949880

- Molecule 56 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	1y	74	Total	C	N	O	P	S	0	0
			1585	707	285	518	74	1		
56	2y	73	Total	C	N	O	P	S	0	0
			1565	698	283	510	73	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	2a	281	Total	Mg	0	0
			281	281		
57	1A	1297	Total	Mg	0	0
			1297	1297		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	2A	963	Total 963	Mg 963	0	0
57	1a	255	Total 255	Mg 255	0	0

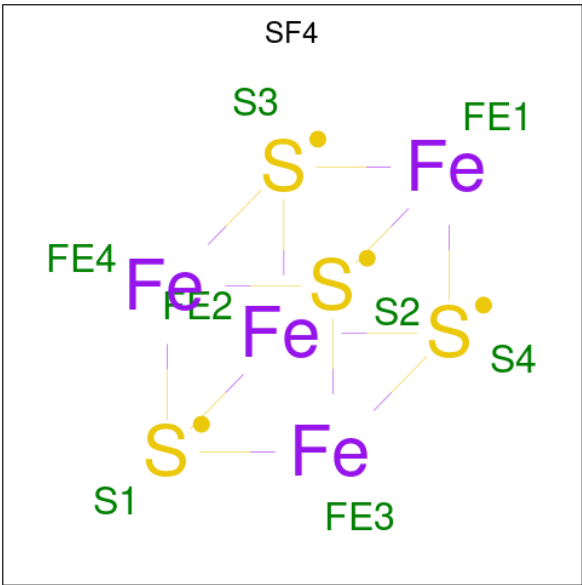
- Molecule 58 is POTASSIUM ION (three-letter code: K) (formula: K).

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
59	14	1	Total 1	Zn 1	0	0
59	1n	1	Total 1	Zn 1	0	0
59	15	1	Total 1	Zn 1	0	0
59	29	1	Total 1	Zn 1	0	0
59	19	1	Total 1	Zn 1	0	0
59	26	1	Total 1	Zn 1	0	0
59	25	1	Total 1	Zn 1	0	0
59	24	1	Total 1	Zn 1	0	0
59	2n	1	Total 1	Zn 1	0	0
59	2Y	1	Total 1	Zn 1	0	0
59	16	1	Total 1	Zn 1	0	0

- Molecule 60 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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		

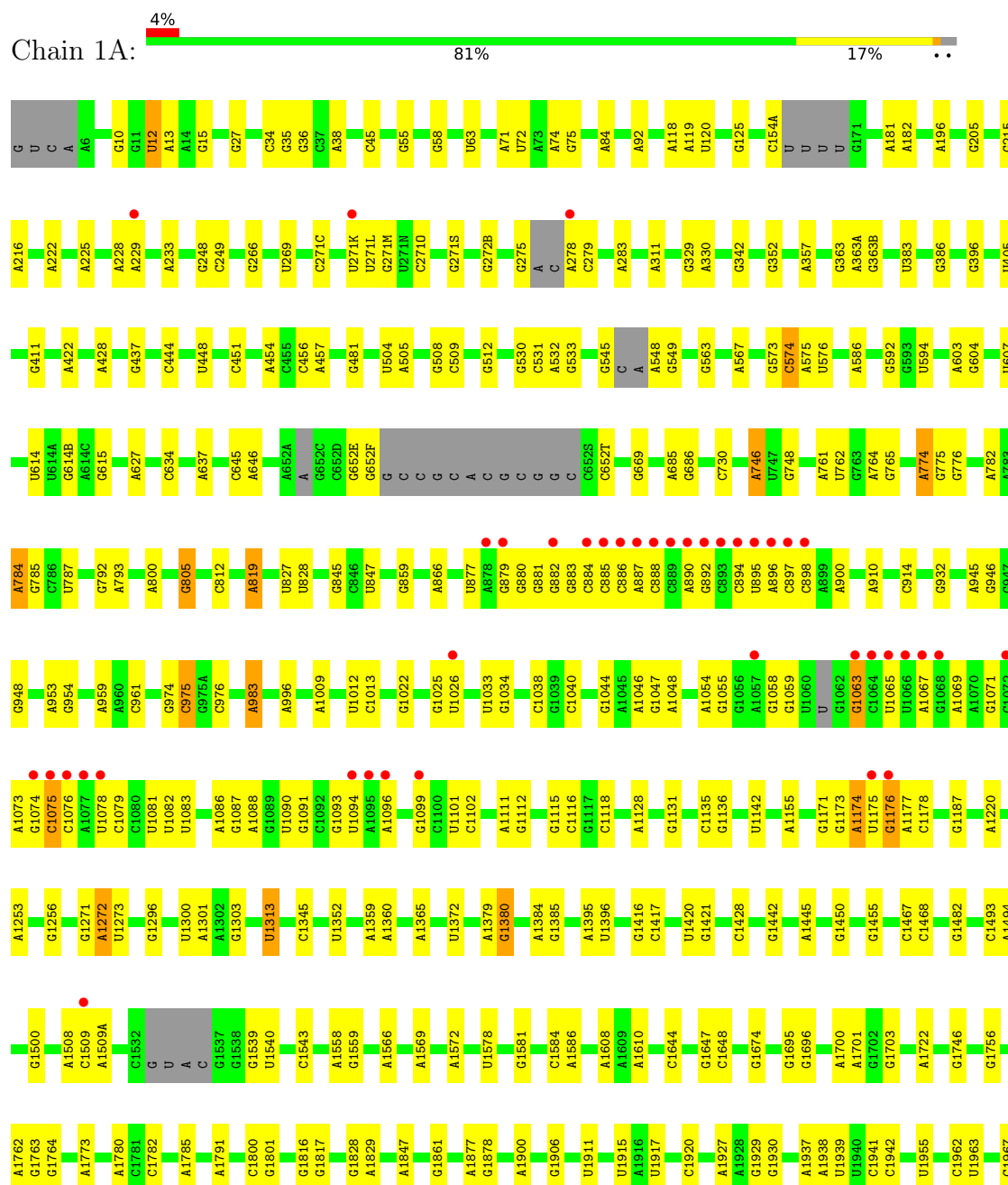
- Molecule 61 is water.

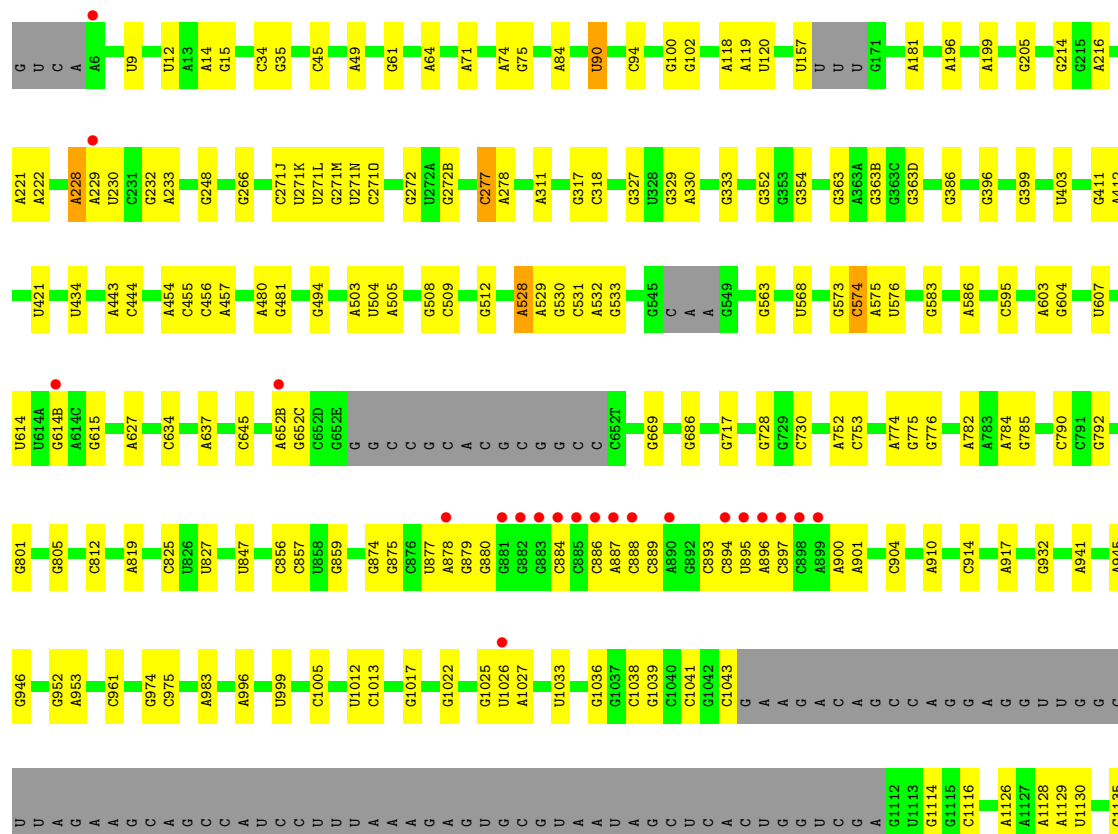
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	2319	Total	O	0	0
			2319	2319		
61	1a	422	Total	O	0	0
			422	422		
61	2A	1298	Total	O	0	0
			1298	1298		
61	2a	304	Total	O	0	0
			304	304		

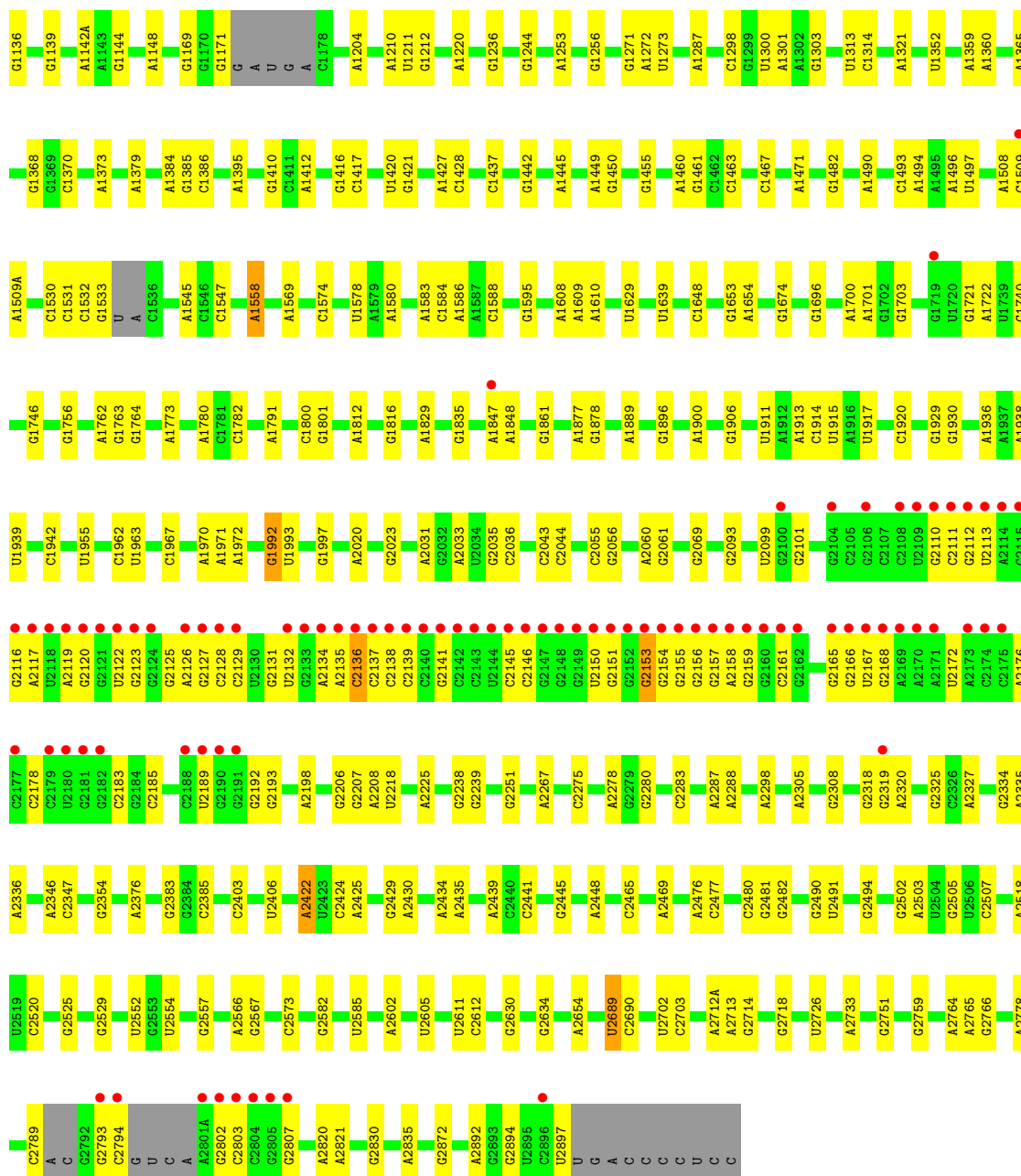
3 Residue-property plots

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







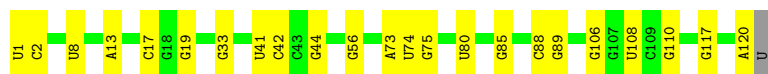
• Molecule 2: 5S Ribosomal RNA

Chain 1B: 90% 9%

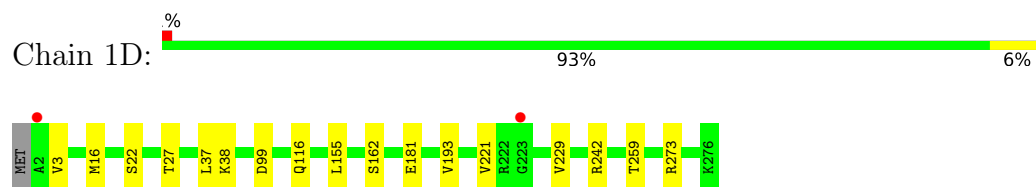


• Molecule 2: 5S Ribosomal RNA

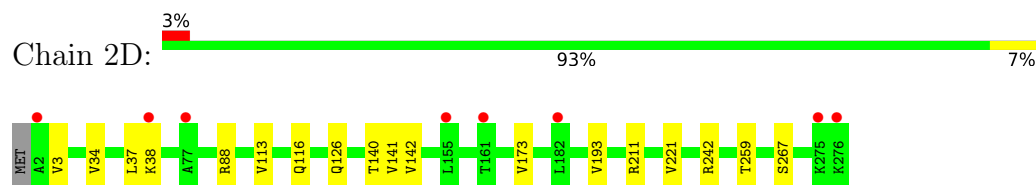
Chain 2B: 80% 19%



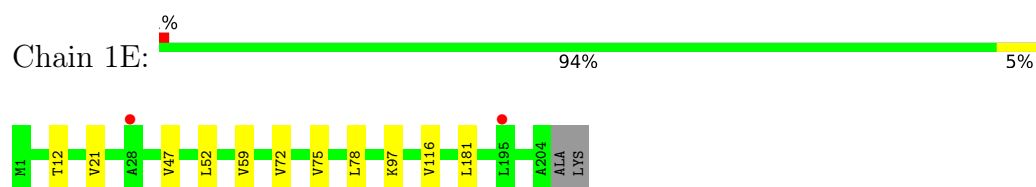
• Molecule 3: 50S ribosomal protein L2



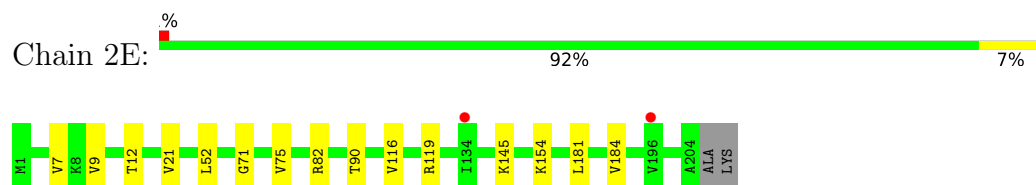
• Molecule 3: 50S ribosomal protein L2



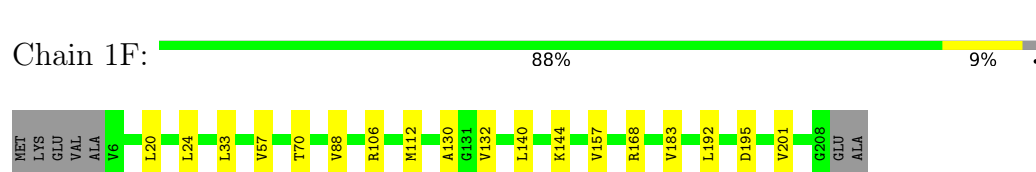
• Molecule 4: 50S ribosomal protein L3



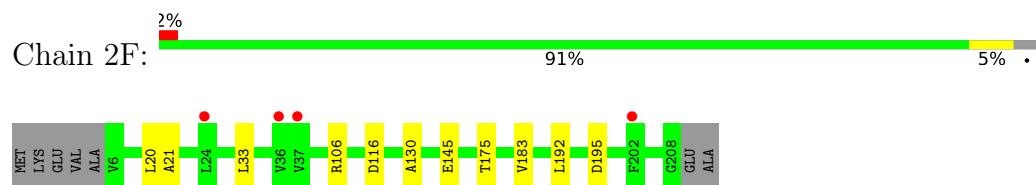
• Molecule 4: 50S ribosomal protein L3



• Molecule 5: 50S ribosomal protein L4



• Molecule 5: 50S ribosomal protein L4

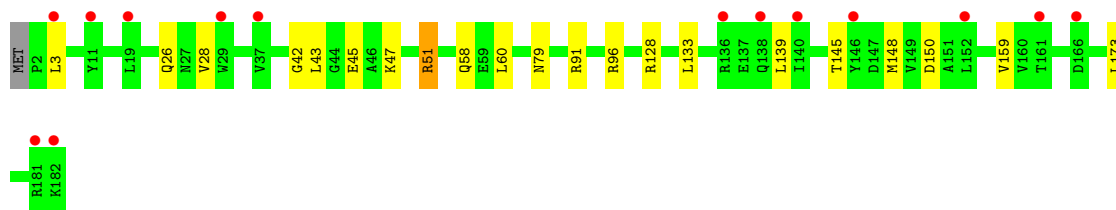
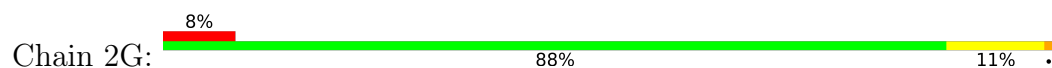


• Molecule 6: 50S ribosomal protein L5





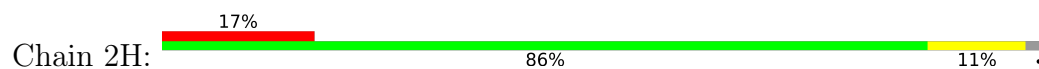
- Molecule 6: 50S ribosomal protein L5



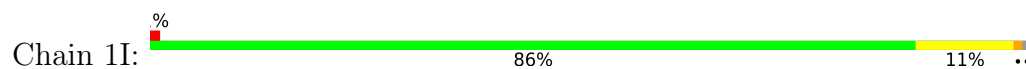
- Molecule 7: 50S ribosomal protein L6



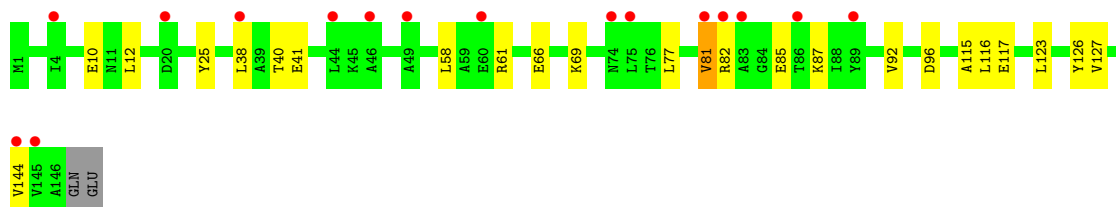
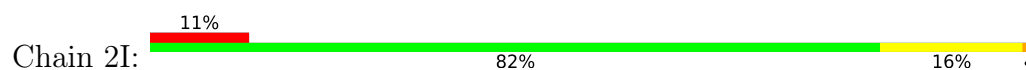
- Molecule 7: 50S ribosomal protein L6



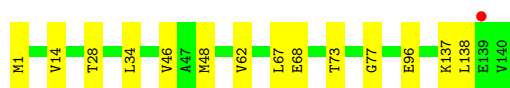
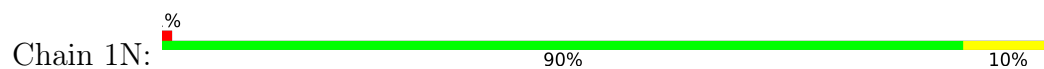
- Molecule 8: 50S ribosomal protein L9



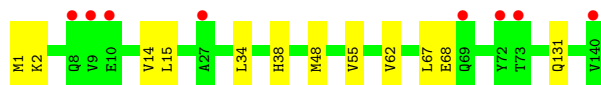
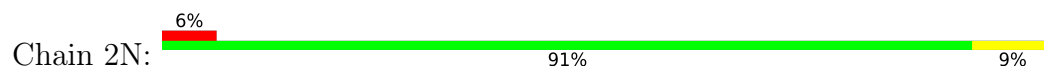
- Molecule 8: 50S ribosomal protein L9



• Molecule 9: 50S ribosomal protein L13



• Molecule 9: 50S ribosomal protein L13



• Molecule 10: 50S ribosomal protein L14



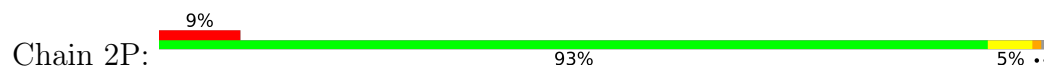
• Molecule 10: 50S ribosomal protein L14



• Molecule 11: 50S ribosomal protein L15



• Molecule 11: 50S ribosomal protein L15

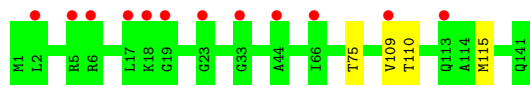


• Molecule 12: 50S ribosomal protein L16





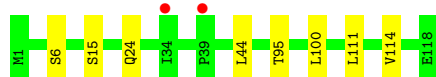
- Molecule 12: 50S ribosomal protein L16



- Molecule 13: 50S ribosomal protein L17



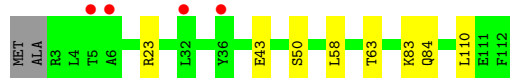
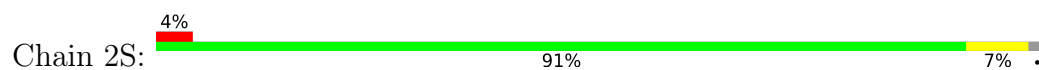
- Molecule 13: 50S ribosomal protein L17



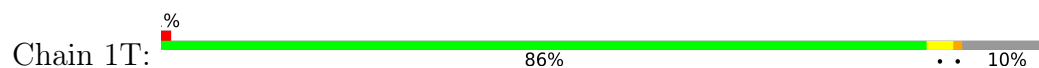
- Molecule 14: 50S ribosomal protein L18



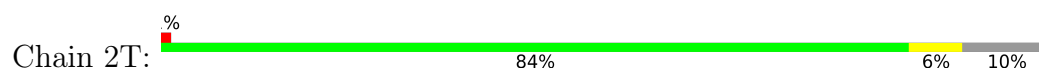
- Molecule 14: 50S ribosomal protein L18



- Molecule 15: 50S ribosomal protein L19



- Molecule 15: 50S ribosomal protein L19



- Molecule 16: 50S ribosomal protein L20



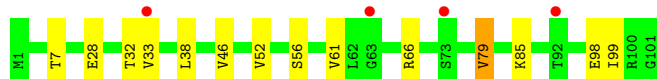
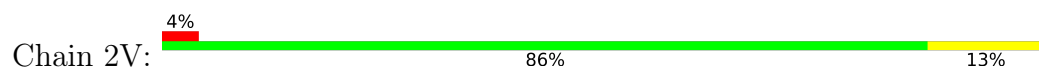
- Molecule 16: 50S ribosomal protein L20



- Molecule 17: 50S ribosomal protein L21



- Molecule 17: 50S ribosomal protein L21



- Molecule 18: 50S ribosomal protein L22

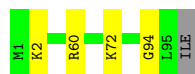


- Molecule 18: 50S ribosomal protein L22



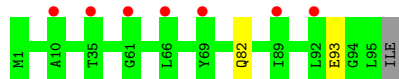
- Molecule 19: 50S ribosomal protein L23

Chain 1X:  95% ..



- Molecule 19: 50S ribosomal protein L23

Chain 2X:  7% 97% ..




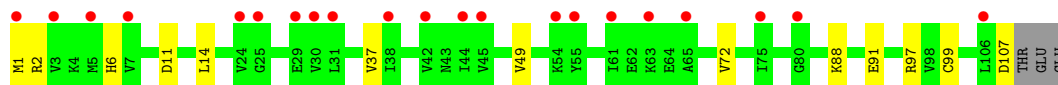
- Molecule 20: 50S ribosomal protein L24

Chain 1Y:  89% 8% .



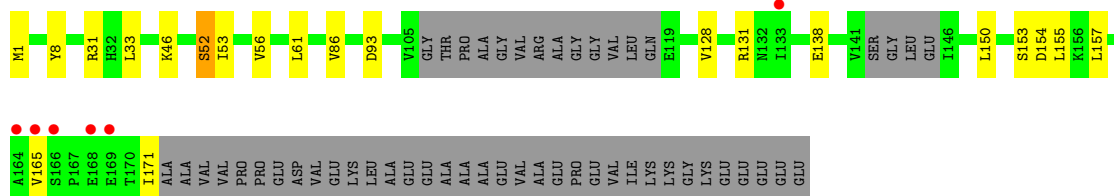
- Molecule 20: 50S ribosomal protein L24

Chain 2Y:  19% 85% 12% .



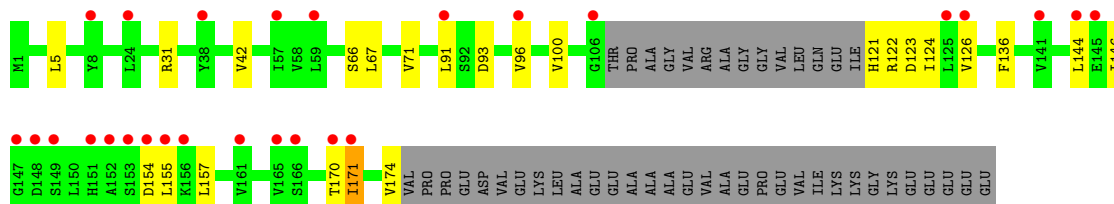
- Molecule 21: 50S ribosomal protein L25

Chain 1Z:  3% 65% 10% 25%



- Molecule 21: 50S ribosomal protein L25

Chain 2Z:  13% 66% 11% 22%



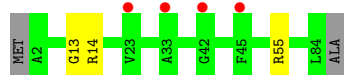
- Molecule 22: 50S ribosomal protein L27

Chain 10:  95% ..



- Molecule 22: 50S ribosomal protein L27

Chain 20:  5% 94% ..



- Molecule 23: 50S ribosomal protein L28

Chain 11:  3% 94% 5% .



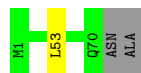
- Molecule 23: 50S ribosomal protein L28

Chain 21:  6% 95% ..



- Molecule 24: 50S ribosomal protein L29

Chain 12:  96% ..



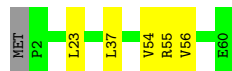
- Molecule 24: 50S ribosomal protein L29

Chain 22:  94% ..

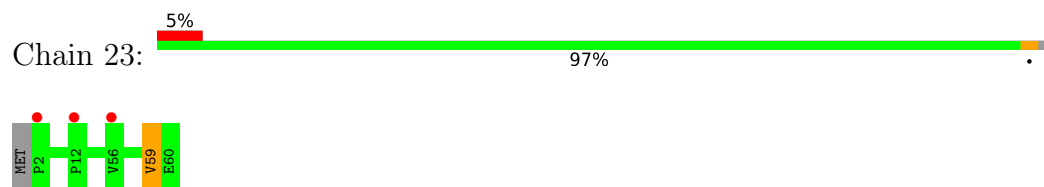


- Molecule 25: 50S ribosomal protein L30

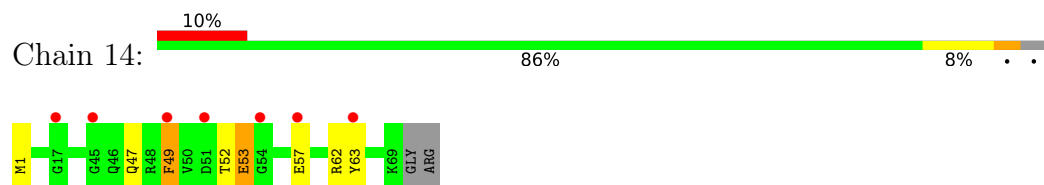
Chain 13:  90% 8% .



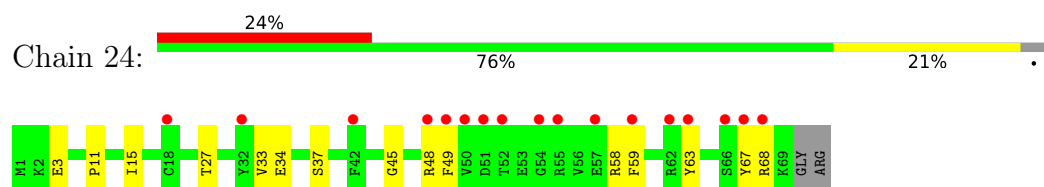
- Molecule 25: 50S ribosomal protein L30



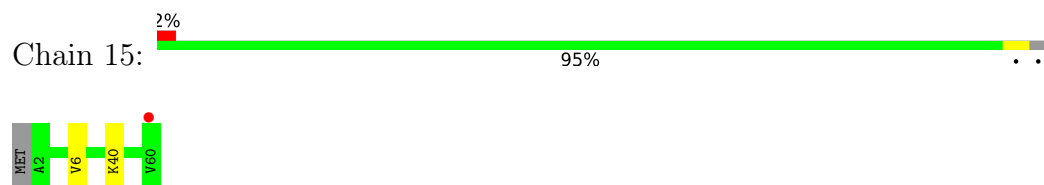
- Molecule 26: 50S ribosomal protein L31



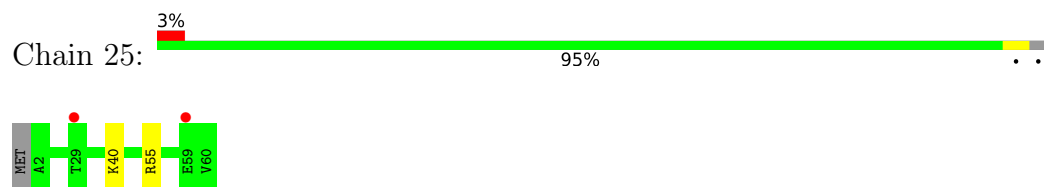
- Molecule 26: 50S ribosomal protein L31



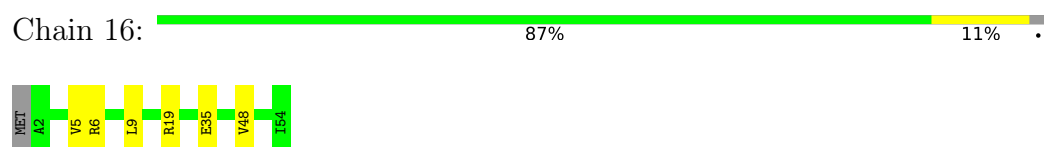
- Molecule 27: 50S ribosomal protein L32



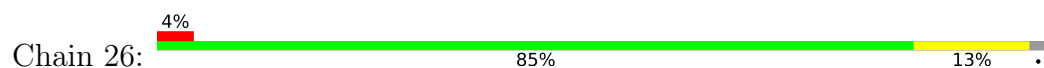
- Molecule 27: 50S ribosomal protein L32

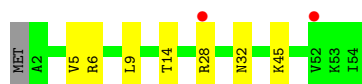


- Molecule 28: 50S ribosomal protein L33

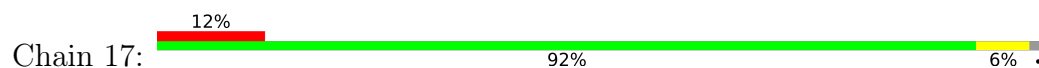


- Molecule 28: 50S ribosomal protein L33

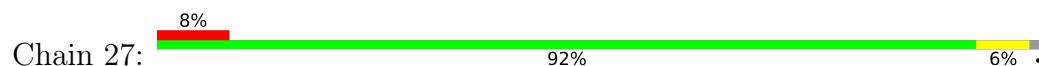




- Molecule 29: 50S ribosomal protein L34



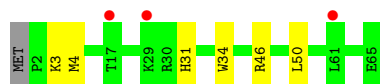
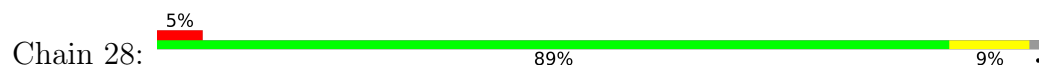
- Molecule 29: 50S ribosomal protein L34



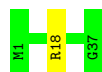
- Molecule 30: 50S ribosomal protein L35



- Molecule 30: 50S ribosomal protein L35



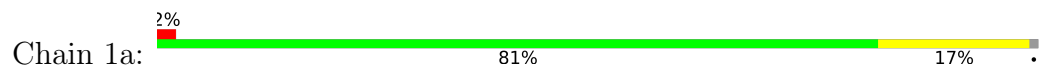
- Molecule 31: 50S ribosomal protein L36

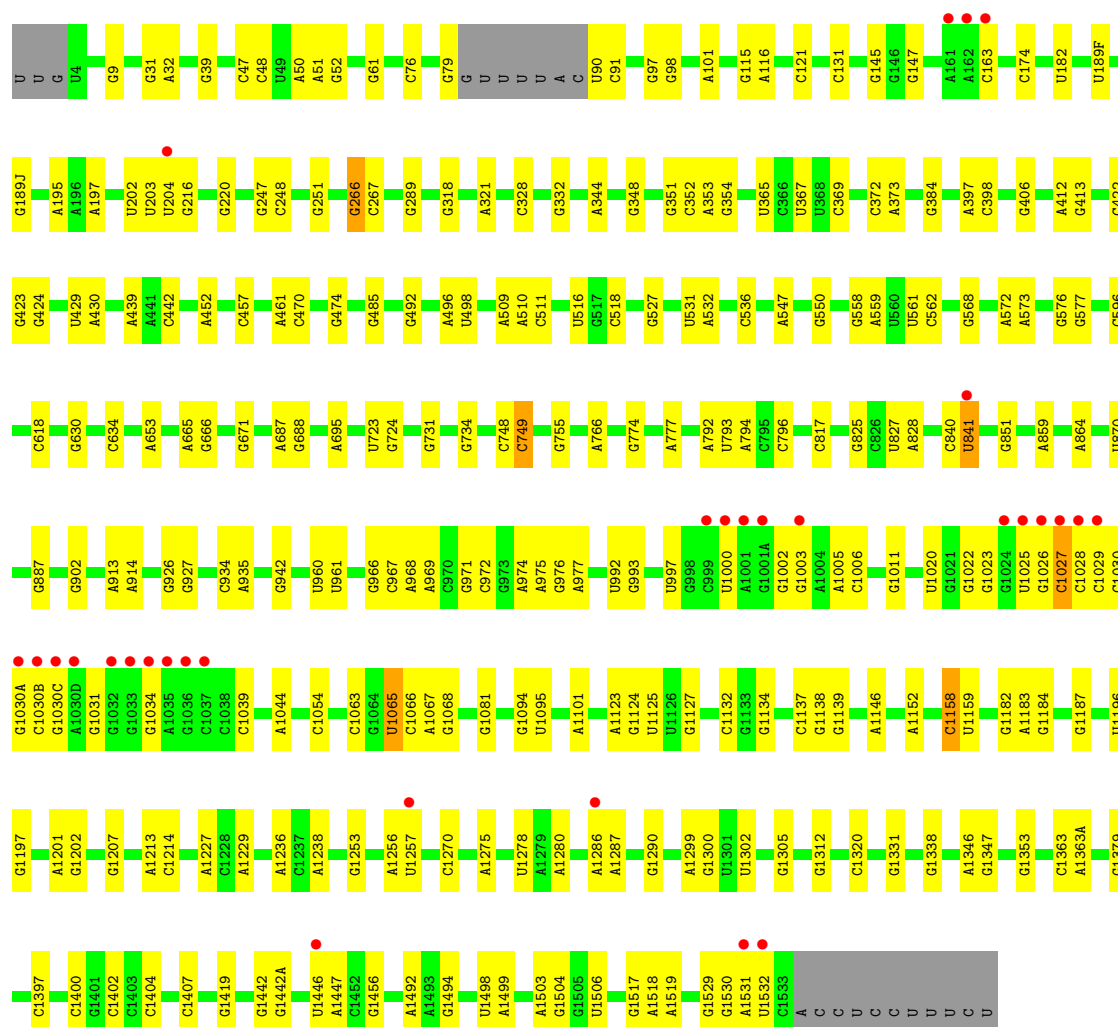


- Molecule 31: 50S ribosomal protein L36



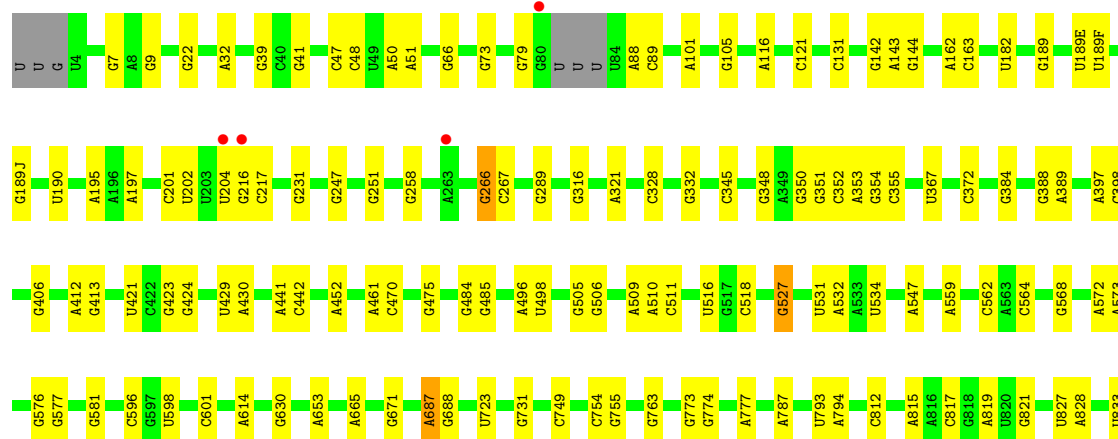
- Molecule 32: 16S Ribosomal RNA

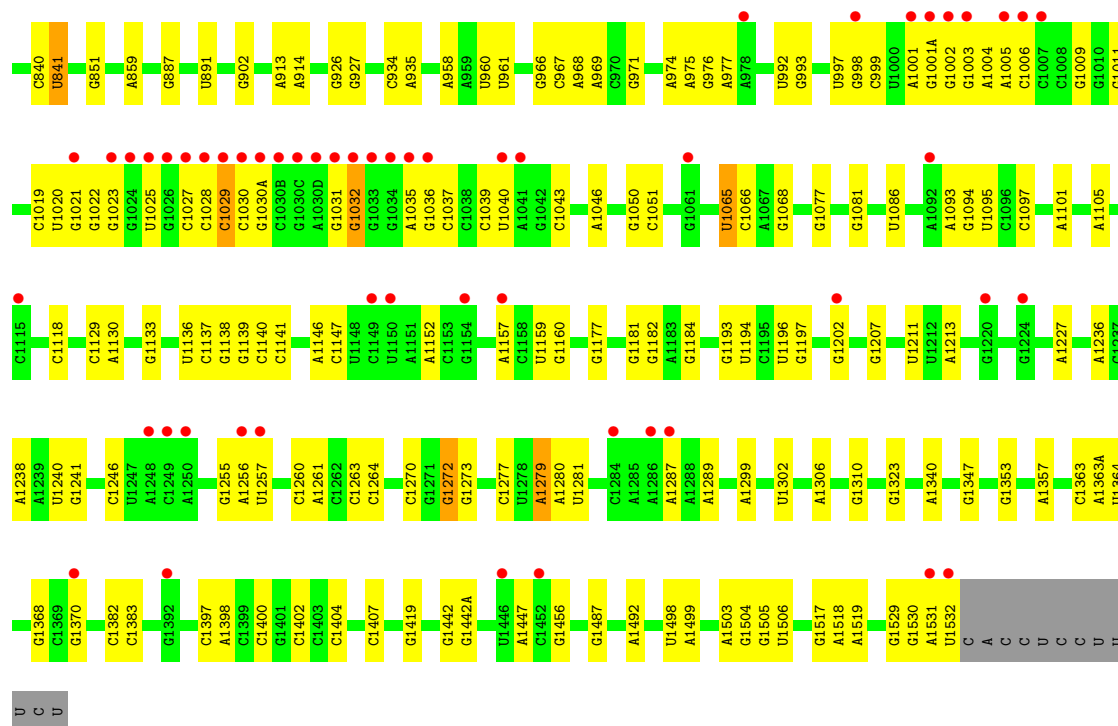




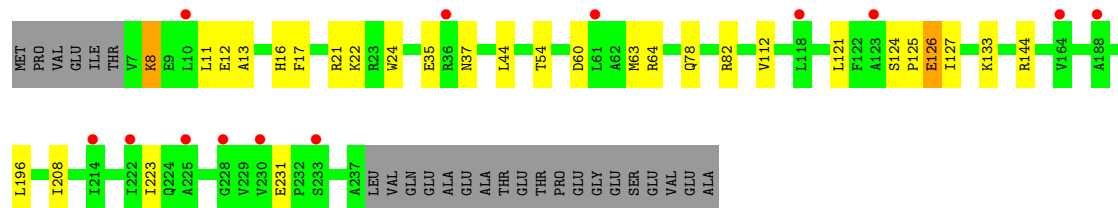
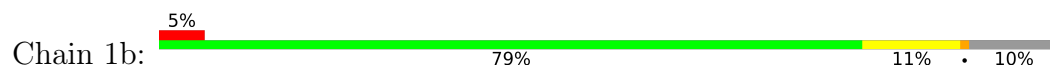
• Molecule 32: 16S Ribosomal RNA

Chain 2a: 4% 79% 19% ::

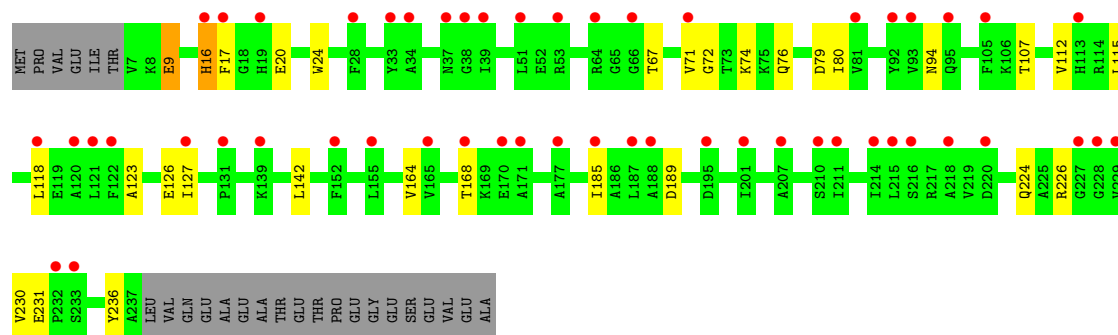
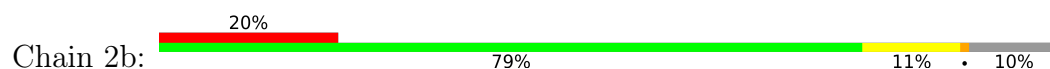




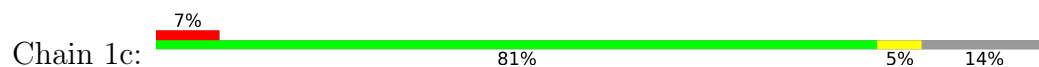
• Molecule 33: 30S ribosomal protein S2

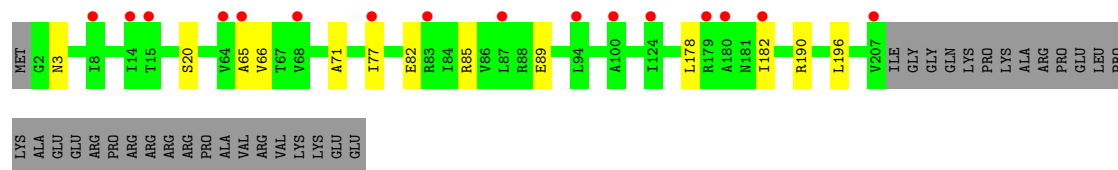


• Molecule 33: 30S ribosomal protein S2

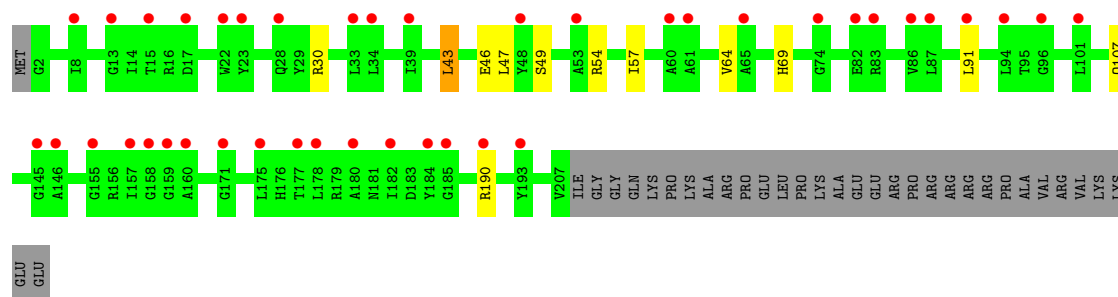
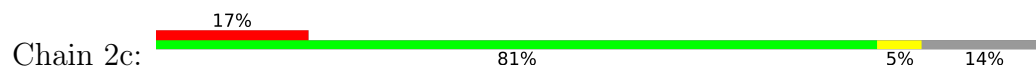


• Molecule 34: 30S ribosomal protein S3





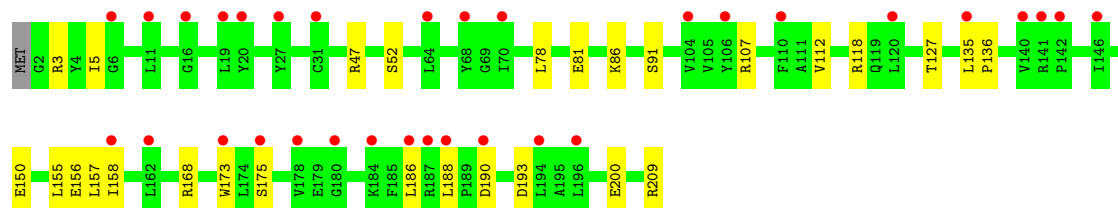
- Molecule 34: 30S ribosomal protein S3



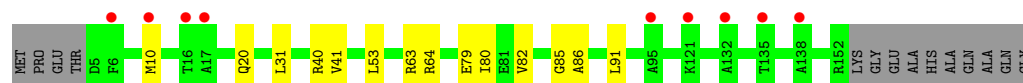
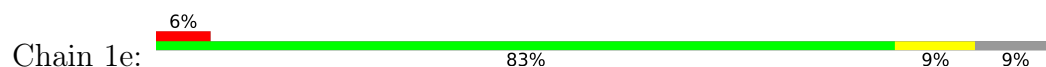
- Molecule 35: 30S ribosomal protein S4



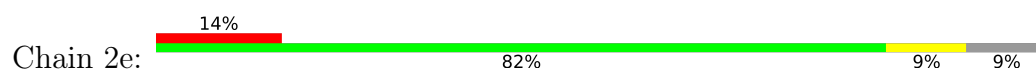
- Molecule 35: 30S ribosomal protein S4

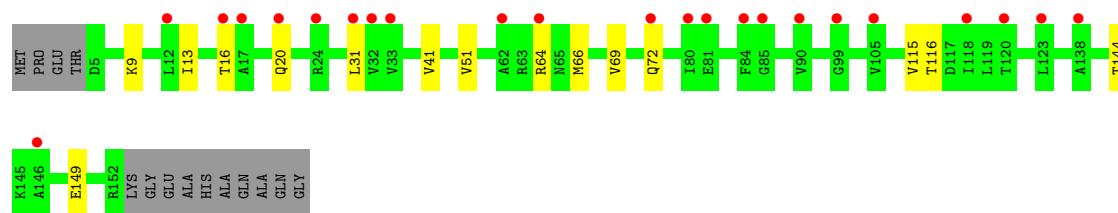


- Molecule 36: 30S ribosomal protein S5

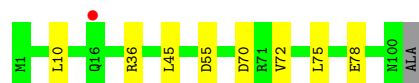
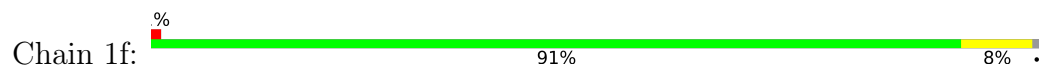


- Molecule 36: 30S ribosomal protein S5

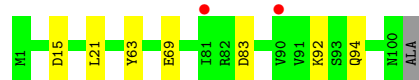
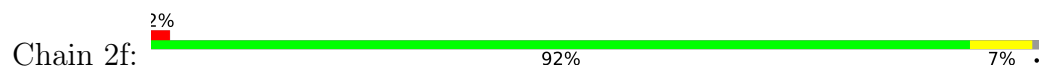




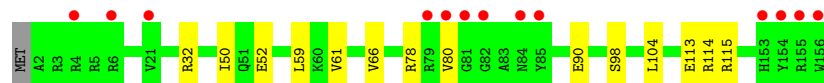
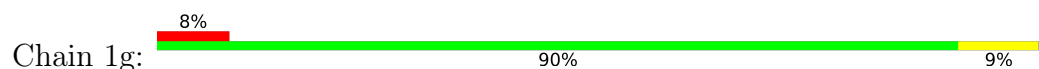
- Molecule 37: 30S ribosomal protein S6



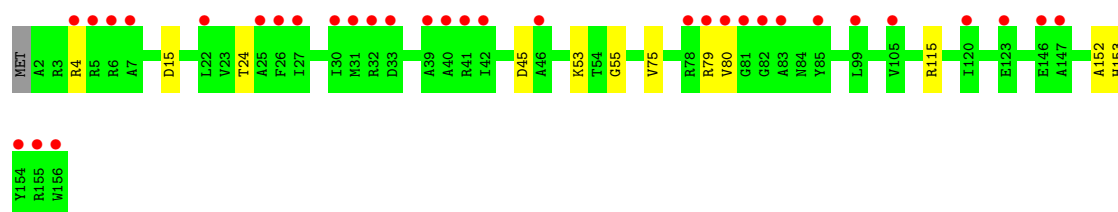
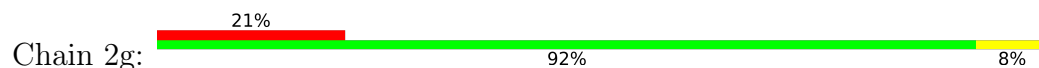
- Molecule 37: 30S ribosomal protein S6



- Molecule 38: 30S ribosomal protein S7



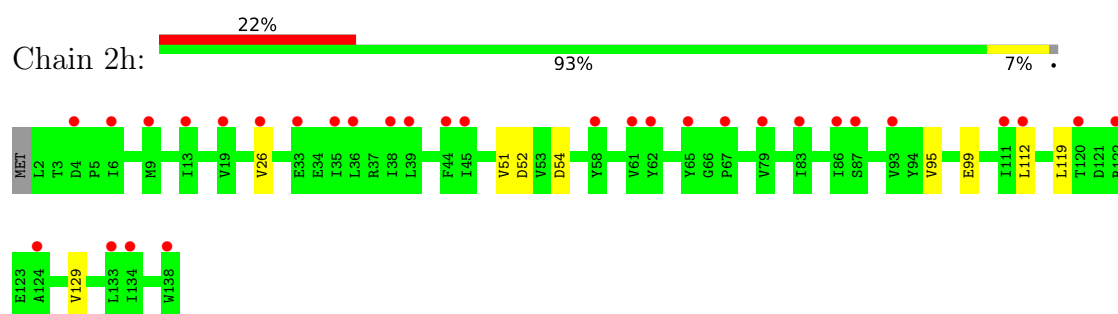
- Molecule 38: 30S ribosomal protein S7



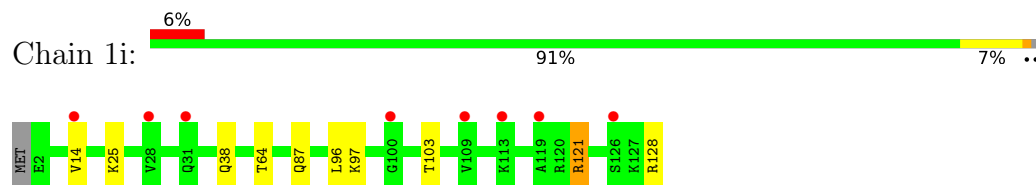
- Molecule 39: 30S ribosomal protein S8



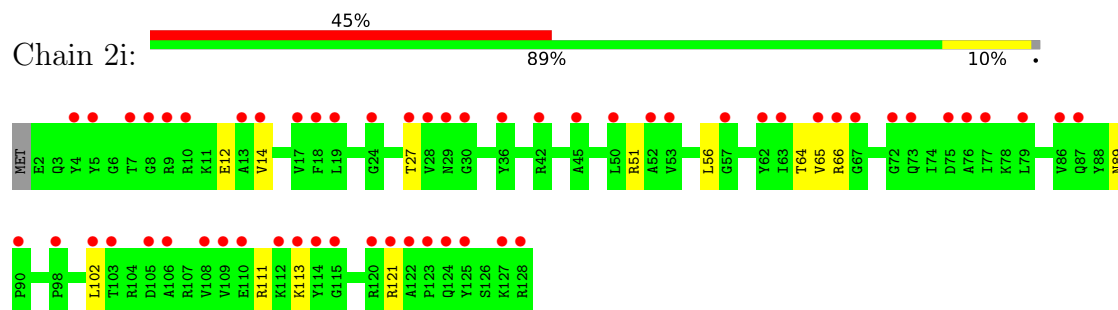
- Molecule 39: 30S ribosomal protein S8



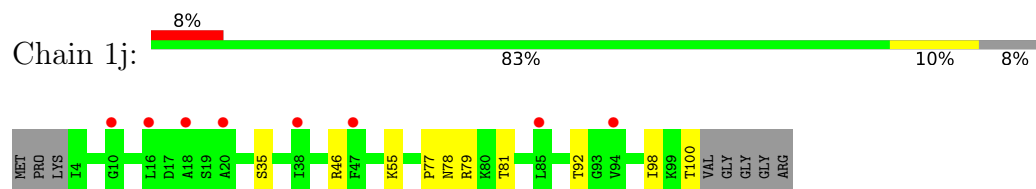
- Molecule 40: 30S ribosomal protein S9



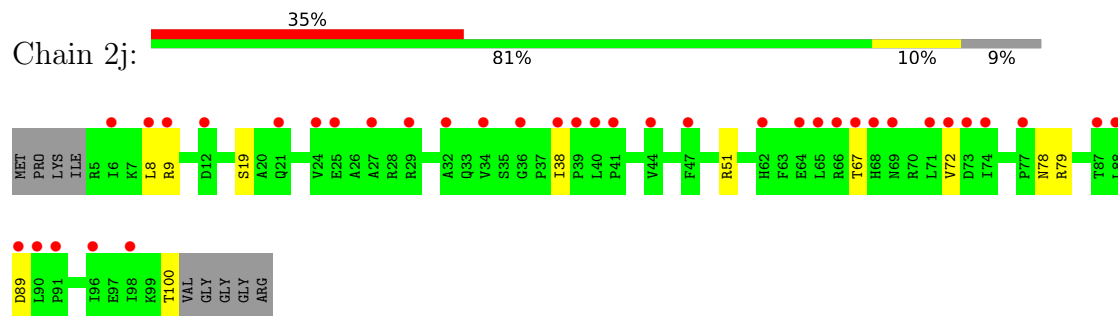
- Molecule 40: 30S ribosomal protein S9



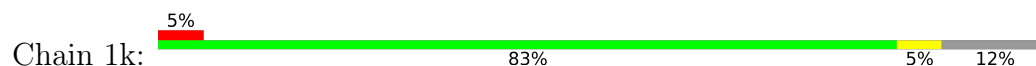
- Molecule 41: 30S ribosomal protein S10

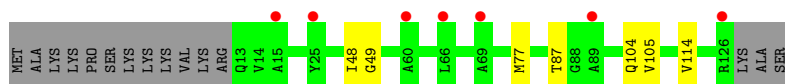


- Molecule 41: 30S ribosomal protein S10

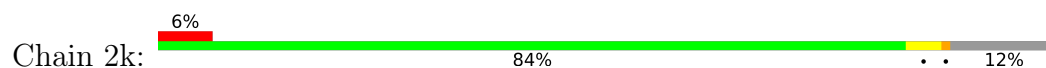


- Molecule 42: 30S ribosomal protein S11

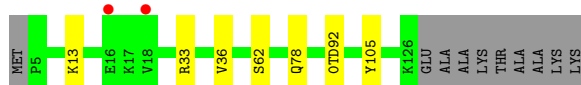
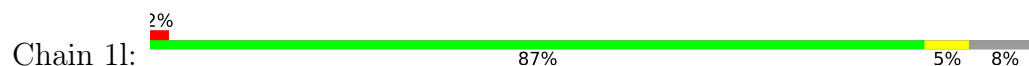




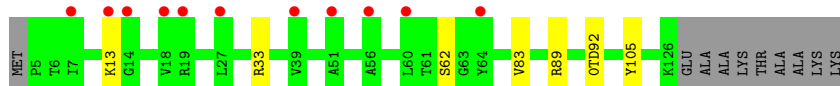
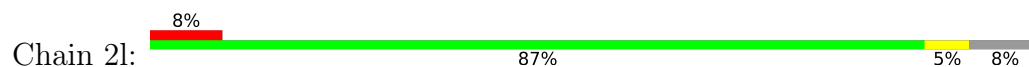
- Molecule 42: 30S ribosomal protein S11



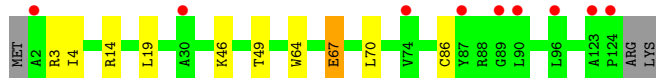
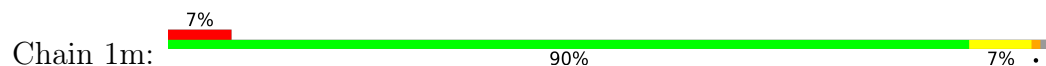
- Molecule 43: 30S ribosomal protein S12



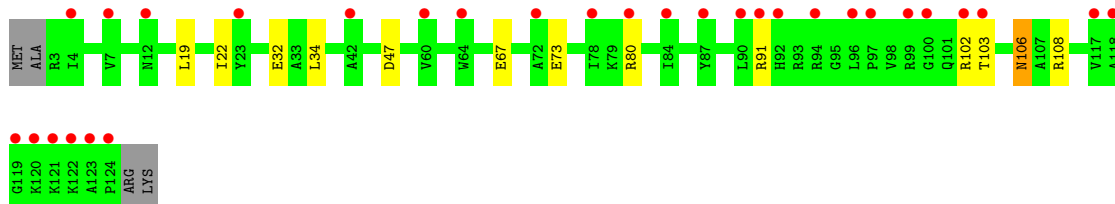
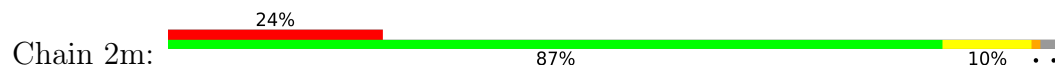
- Molecule 43: 30S ribosomal protein S12



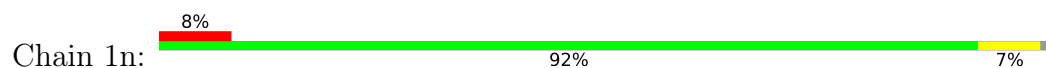
- Molecule 44: 30S ribosomal protein S13

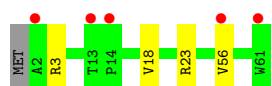


- Molecule 44: 30S ribosomal protein S13

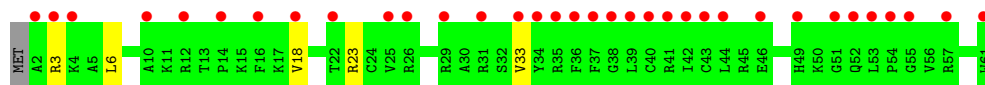
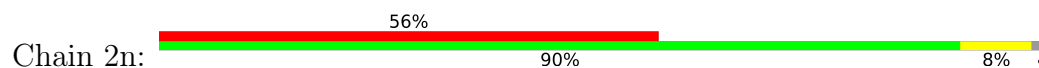


- Molecule 45: 30S ribosomal protein S14 type Z

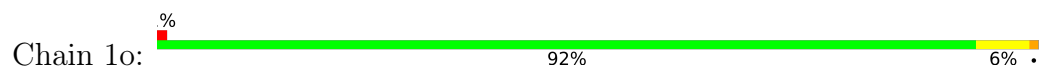




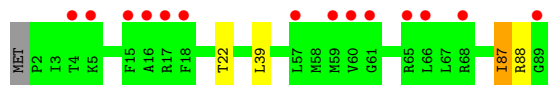
- Molecule 45: 30S ribosomal protein S14 type Z



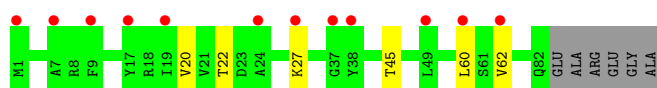
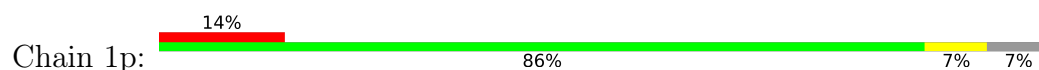
- Molecule 46: 30S ribosomal protein S15



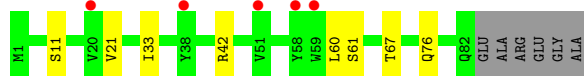
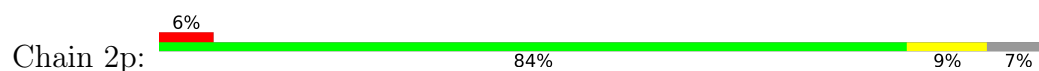
- Molecule 46: 30S ribosomal protein S15



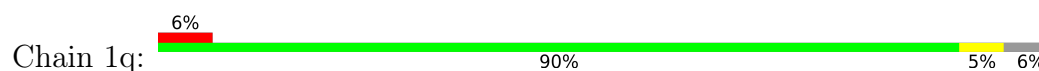
- Molecule 47: 30S ribosomal protein S16



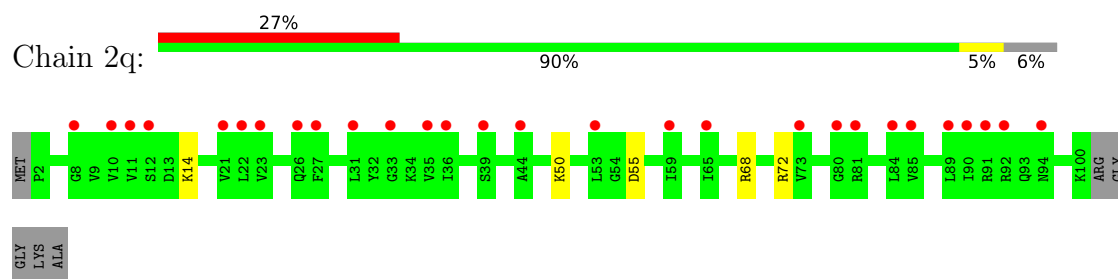
- Molecule 47: 30S ribosomal protein S16



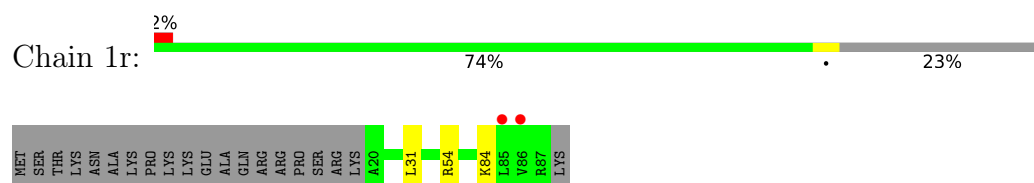
- Molecule 48: 30S ribosomal protein S17



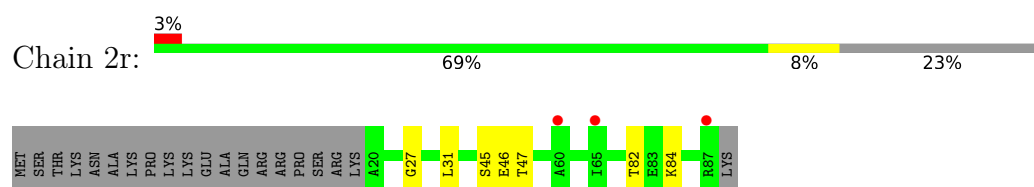
- Molecule 48: 30S ribosomal protein S17



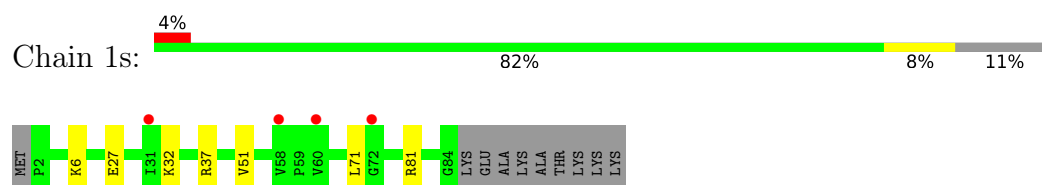
- Molecule 49: 30S ribosomal protein S18



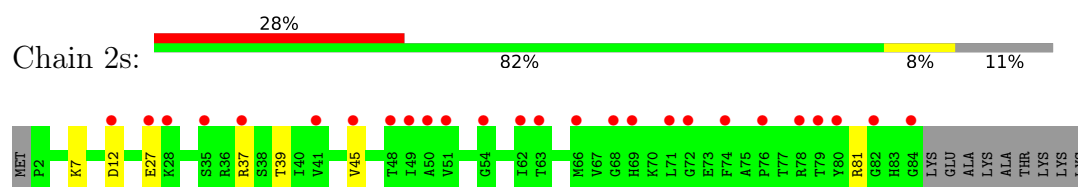
- Molecule 49: 30S ribosomal protein S18



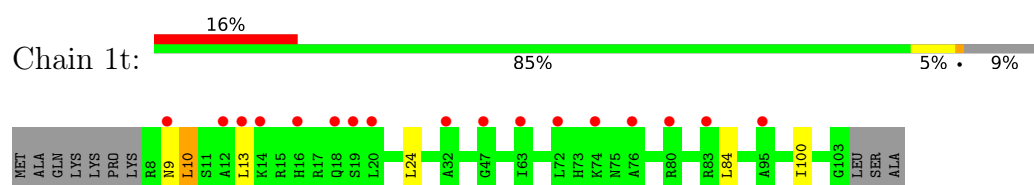
- Molecule 50: 30S ribosomal protein S19



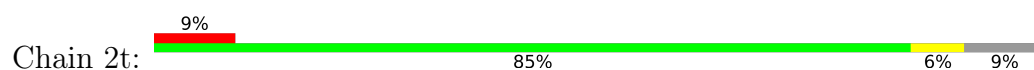
- Molecule 50: 30S ribosomal protein S19

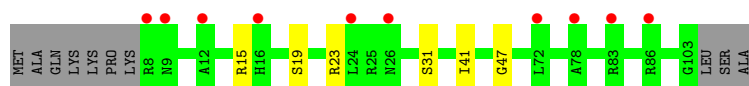


- Molecule 51: 30S ribosomal protein S20

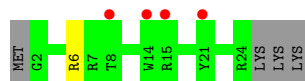
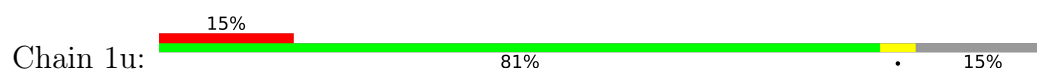


- Molecule 51: 30S ribosomal protein S20

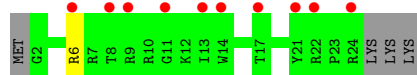
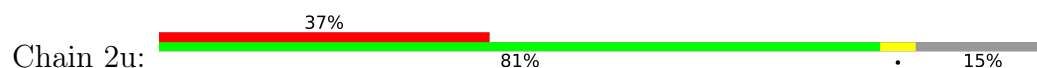




- Molecule 52: 30S ribosomal protein Thx



- Molecule 52: 30S ribosomal protein Thx



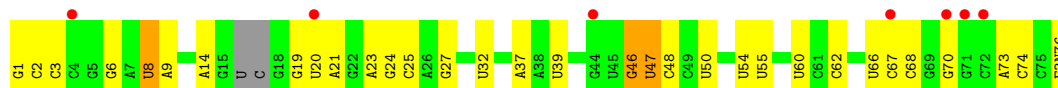
- Molecule 53: mRNA



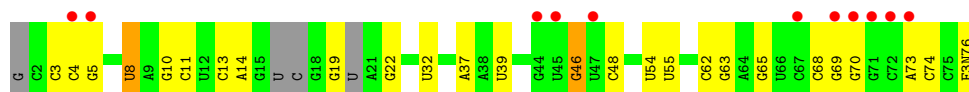
- Molecule 53: mRNA




- Molecule 54: A-site tRNA

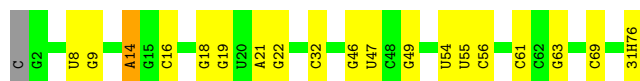


- Molecule 54: A-site tRNA




- Molecule 55: P-site tRNA

Chain 1x:  74% 23% ..




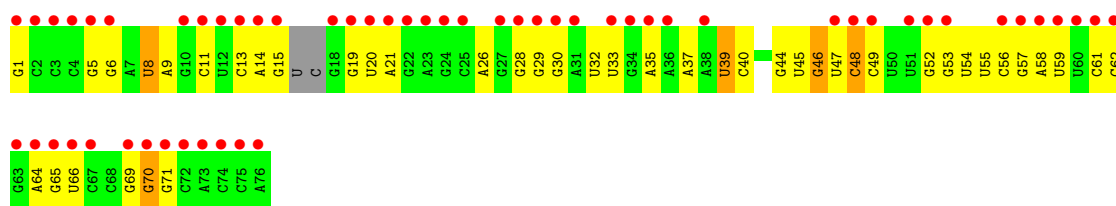
• Molecule 55: P-site tRNA

Chain 2x:  75% 23% .




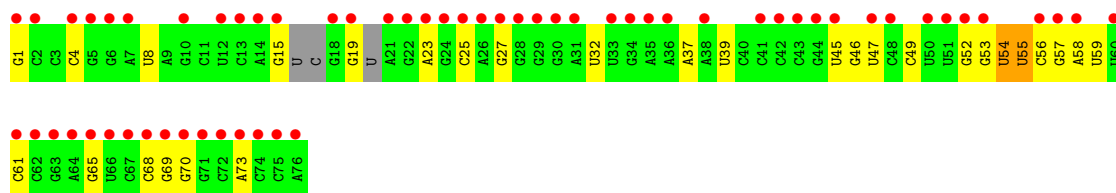
• Molecule 56: E-site tRNA

Chain 1y:  39% 74% 51% 7% .



• Molecule 56: E-site tRNA

Chain 2y:  58% 79% 36% . .



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.83Å 448.31Å 622.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	311.28 – 2.50 311.28 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.3 (311.28-2.50) 97.3 (311.28-2.50)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 2.52Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.233 , 0.281 0.233 , 0.281	Depositor DCC
R_{free} test set	97365 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	46.8	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 50.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	300196	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.64% 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: 5MU, ZN, 4SU, OMG, 2MU, MIA, 31H, SF4, 0TD, MG, F3N, 2MA, 2MG, 5MC, UR3, MA6, 4OC, M2G, 7MG, K, PSU

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	0.53	0/69009	1.03	88/107712 (0.1%)
1	2A	0.41	0/67293	0.90	35/105034 (0.0%)
2	1B	0.49	1/2882 (0.0%)	0.92	0/4494
2	2B	0.42	1/2879 (0.0%)	0.87	1/4487 (0.0%)
3	1D	0.37	0/2186	0.58	0/2944
3	2D	0.32	0/2186	0.53	0/2944
4	1E	0.34	0/1592	0.54	0/2149
4	2E	0.30	0/1592	0.52	0/2149
5	1F	0.35	0/1619	0.54	0/2193
5	2F	0.29	0/1615	0.50	0/2188
6	1G	0.30	0/1448	0.51	0/1957
6	2G	0.30	0/1453	0.51	1/1963 (0.1%)
7	1H	0.31	0/1356	0.50	0/1834
7	2H	0.30	0/1356	0.45	0/1834
8	1I	0.29	0/1112	0.51	0/1514
8	2I	0.31	0/1079	0.50	0/1475
9	1N	0.34	0/1144	0.53	1/1543 (0.1%)
9	2N	0.28	0/1144	0.45	0/1543
10	1O	0.35	0/943	0.55	0/1269
10	2O	0.33	0/943	0.53	0/1269
11	1P	0.34	0/1152	0.58	1/1533 (0.1%)
11	2P	0.31	0/1152	0.51	0/1533
12	1Q	0.36	0/1143	0.55	0/1527
12	2Q	0.31	0/1143	0.48	0/1527
13	1R	0.34	0/982	0.55	0/1312
13	2R	0.29	0/982	0.52	0/1312
14	1S	0.31	0/883	0.52	0/1176
14	2S	0.30	0/880	0.50	0/1172
15	1T	0.33	0/1105	0.53	0/1477
15	2T	0.30	0/1097	0.49	0/1468
16	1U	0.37	0/977	0.54	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.30	0/977	0.46	0/1301
17	1V	0.37	0/782	0.55	0/1049
17	2V	0.31	0/782	0.52	0/1049
18	1W	0.35	0/897	0.54	0/1205
18	2W	0.30	0/897	0.51	0/1205
19	1X	0.37	0/764	0.55	0/1025
19	2X	0.31	0/764	0.52	0/1025
20	1Y	0.33	0/819	0.55	0/1095
20	2Y	0.31	0/819	0.53	0/1095
21	1Z	0.32	0/1267	0.55	0/1717
21	2Z	0.31	0/1299	0.51	0/1763
22	10	0.39	0/662	0.59	0/881
22	20	0.34	0/662	0.53	0/881
23	11	0.34	0/762	0.53	0/1014
23	21	0.30	0/762	0.52	0/1014
24	12	0.31	0/590	0.49	0/781
24	22	0.30	0/590	0.41	0/781
25	13	0.32	0/474	0.54	0/635
25	23	0.29	0/469	0.46	0/630
26	14	0.31	0/565	0.54	0/761
26	24	0.30	0/545	0.47	0/737
27	15	0.36	0/469	0.56	0/635
27	25	0.31	0/469	0.55	0/635
28	16	0.34	0/460	0.54	0/613
28	26	0.29	0/456	0.48	0/608
29	17	0.35	0/426	0.55	0/561
29	27	0.30	0/426	0.48	0/561
30	18	0.33	0/525	0.53	0/691
30	28	0.29	0/525	0.45	0/691
31	19	0.35	0/310	0.57	0/407
31	29	0.31	0/310	0.49	0/407
32	1a	0.39	0/35795	0.92	31/55864 (0.1%)
32	2a	0.37	2/35886 (0.0%)	0.90	38/56005 (0.1%)
33	1b	0.30	0/1881	0.51	0/2542
33	2b	0.30	0/1860	0.50	0/2518
34	1c	0.29	0/1572	0.50	0/2126
34	2c	0.29	0/1566	0.50	1/2119 (0.0%)
35	1d	0.29	0/1685	0.48	0/2262
35	2d	0.28	0/1704	0.46	0/2284
36	1e	0.30	0/1145	0.51	0/1543
36	2e	0.29	0/1149	0.49	0/1548
37	1f	0.30	0/823	0.50	0/1115
37	2f	0.29	0/829	0.47	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.28	0/1250	0.43	0/1679
38	2g	0.28	0/1254	0.45	0/1683
39	1h	0.29	0/1108	0.49	0/1494
39	2h	0.28	0/1108	0.46	0/1494
40	1i	0.30	0/1002	0.57	1/1346 (0.1%)
40	2i	0.30	0/997	0.50	0/1343
41	1j	0.29	0/722	0.50	0/982
41	2j	0.28	0/727	0.52	0/988
42	1k	0.30	0/844	0.50	0/1145
42	2k	0.30	0/848	0.47	0/1149
43	1l	0.31	0/937	0.52	0/1260
43	2l	0.28	0/937	0.49	0/1260
44	1m	0.30	0/969	0.49	0/1302
44	2m	0.29	0/961	0.50	0/1291
45	1n	0.31	0/501	0.49	0/664
45	2n	0.30	0/501	0.47	0/664
46	1o	0.28	0/739	0.45	0/985
46	2o	0.28	0/739	0.45	0/985
47	1p	0.28	0/697	0.49	0/939
47	2p	0.26	0/693	0.50	0/935
48	1q	0.30	0/836	0.49	0/1117
48	2q	0.30	0/836	0.49	0/1117
49	1r	0.29	0/560	0.48	0/746
49	2r	0.27	0/560	0.48	0/746
50	1s	0.29	0/667	0.56	0/900
50	2s	0.30	0/661	0.55	0/893
51	1t	0.28	0/730	0.47	0/965
51	2t	0.32	0/729	0.46	0/965
52	1u	0.27	0/203	0.48	0/266
52	2u	0.26	0/203	0.48	0/266
53	1v	0.48	0/310	0.84	0/480
53	2v	0.40	0/310	0.94	0/480
54	1w	0.53	1/1581 (0.1%)	1.12	4/2458 (0.2%)
54	2w	0.44	0/1531	1.07	2/2379 (0.1%)
55	1x	0.57	3/1700 (0.2%)	1.19	21/2650 (0.8%)
55	2x	0.47	2/1700 (0.1%)	1.09	16/2650 (0.6%)
56	1y	0.60	1/1606 (0.1%)	1.21	9/2497 (0.4%)
56	2y	0.55	1/1583 (0.1%)	1.10	1/2459 (0.0%)
All	All	0.41	12/316586 (0.0%)	0.86	251/473957 (0.1%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	1	G	OP3-P	-10.44	1.48	1.61
56	1y	1	G	OP3-P	-10.41	1.48	1.61
2	2B	1	U	OP3-P	-10.32	1.48	1.61
2	1B	1	U	OP3-P	-10.13	1.49	1.61
56	2y	1	G	OP3-P	-10.10	1.49	1.61
32	2a	1272	G	N1-C2	-7.58	1.31	1.37
32	2a	1272	G	C6-N1	-6.71	1.34	1.39
55	1x	22	G	N7-C5	6.50	1.43	1.39
55	1x	14	A	N7-C5	-6.32	1.35	1.39
55	1x	14	A	C8-N7	-6.12	1.27	1.31
55	2x	22	G	N7-C5	5.51	1.42	1.39
55	2x	14	A	N7-C5	-5.00	1.36	1.39

All (251) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1263	C	N1-C2-O2	21.26	131.66	118.90
32	2a	1272	G	N3-C2-N2	19.96	133.88	119.90
32	2a	1272	G	C5-C6-O6	15.58	137.95	128.60
32	2a	1272	G	N1-C2-N2	-15.03	102.67	116.20
32	2a	1272	G	C6-N1-C2	13.24	133.04	125.10
32	2a	1263	C	C2-N3-C4	13.08	126.44	119.90
1	1A	1086	A	N1-C6-N6	-11.74	111.56	118.60
32	2a	1263	C	N3-C2-O2	-11.36	113.95	121.90
55	1x	14	A	C4-C5-C6	10.73	122.37	117.00
32	2a	1263	C	C5-C6-N1	10.72	126.36	121.00
1	1A	1075	C	N1-C2-O2	10.59	125.25	118.90
1	1A	1063	G	C5-C6-O6	10.14	134.68	128.60
32	2a	1272	G	C5-C6-N1	-9.96	106.52	111.50
55	1x	46	G	C6-N1-C2	-9.87	119.18	125.10
1	1A	2554	U	O5'-P-OP1	-9.61	97.05	105.70
55	2x	46	G	C6-N1-C2	-9.57	119.36	125.10
55	2x	14	A	C4-C5-C6	9.36	121.68	117.00
32	1a	1030(B)	C	N1-C2-O2	8.99	124.30	118.90
54	1w	47	U	C2-N1-C1'	8.94	128.43	117.70
55	1x	22	G	N1-C6-O6	-8.85	114.59	119.90
32	1a	1030(B)	C	C2-N1-C1'	8.72	128.39	118.80
55	1x	14	A	C5-C6-N1	-8.65	113.37	117.70
1	1A	1075	C	C2-N3-C4	8.46	124.13	119.90
32	2a	1263	C	C2-N1-C1'	8.26	127.89	118.80
32	1a	1034	G	C5-C6-O6	8.23	133.53	128.60
55	1x	14	A	C5-N7-C8	8.12	107.96	103.90
1	2A	576	U	O5'-P-OP1	-8.08	98.43	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1029	C	N1-C2-O2	8.06	123.73	118.90
32	2a	1263	C	C4-C5-C6	-7.92	113.44	117.40
1	1A	576	U	O5'-P-OP1	-7.89	98.59	105.70
32	1a	558	G	O5'-P-OP1	-7.78	98.70	105.70
1	1A	512	G	O4'-C1'-N9	7.77	114.42	108.20
55	1x	22	G	C4-C5-C6	-7.76	114.14	118.80
1	1A	1063	G	N3-C2-N2	7.74	125.31	119.90
1	1A	800	A	O5'-P-OP1	-7.73	98.74	105.70
32	2a	1272	G	C8-N9-C1'	-7.62	117.09	127.00
1	2A	801	G	O5'-P-OP2	-7.59	98.86	105.70
54	1w	47	U	N1-C2-O2	7.55	128.09	122.80
32	2a	1272	G	C4-N9-C1'	7.55	136.31	126.50
1	1A	567	A	O5'-P-OP1	-7.51	98.94	105.70
32	1a	1030(B)	C	N3-C2-O2	-7.41	116.71	121.90
55	1x	22	G	C5-N7-C8	-7.39	100.60	104.30
32	2a	1272	G	N1-C6-O6	-7.31	115.51	119.90
55	2x	22	G	N1-C6-O6	-7.29	115.53	119.90
32	1a	841	U	C5-C6-N1	7.28	126.34	122.70
1	1A	1380	G	O5'-P-OP2	-7.21	99.21	105.70
2	2B	80	U	O4'-C1'-N1	7.15	113.92	108.20
32	1a	1030(B)	C	C6-N1-C2	-7.13	117.45	120.30
32	2a	841	U	C5-C6-N1	7.04	126.22	122.70
1	1A	975	C	N1-C2-O2	-7.03	114.68	118.90
1	1A	2682	U	O5'-P-OP2	-6.99	99.41	105.70
1	1A	1063	G	C6-N1-C2	6.96	129.28	125.10
55	2x	22	G	C4-C5-C6	-6.95	114.63	118.80
1	1A	787	U	O5'-P-OP1	-6.93	99.46	105.70
32	2a	1263	C	N1-C2-N3	-6.93	114.35	119.20
32	1a	1158	C	C2-N1-C1'	6.88	126.36	118.80
1	1A	847	U	C2-N1-C1'	6.83	125.90	117.70
1	1A	1993	U	O5'-P-OP1	-6.83	99.56	105.70
32	2a	1263	C	C6-N1-C2	-6.79	117.58	120.30
1	1A	2015	A	O5'-P-OP1	-6.76	99.61	105.70
1	1A	2577	A	O5'-P-OP1	-6.71	99.66	105.70
55	2x	14	A	C5-N7-C8	6.66	107.23	103.90
1	2A	1298	C	O5'-P-OP2	-6.66	99.71	105.70
32	1a	266	G	P-O3'-C3'	6.60	127.62	119.70
32	1a	1034	G	C6-N1-C2	6.57	129.04	125.10
1	2A	574	C	O5'-P-OP1	-6.55	99.80	105.70
55	1x	22	G	N3-C4-N9	-6.55	122.07	126.00
1	2A	2490	G	C5-C6-O6	-6.55	124.67	128.60
1	1A	954	G	O5'-P-OP1	-6.54	99.81	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2685	G	N1-C6-O6	-6.50	116.00	119.90
1	1A	2593	U	N3-C4-O4	-6.43	114.90	119.40
1	1A	1086	A	C5-C6-N6	6.40	128.82	123.70
1	1A	1992	G	P-O3'-C3'	6.38	127.36	119.70
1	1A	2167	U	C2-N1-C1'	6.35	125.32	117.70
1	1A	1644	C	C2-N1-C1'	6.34	125.78	118.80
55	1x	22	G	C6-C5-N7	6.34	134.21	130.40
1	2A	1639	U	O5'-P-OP2	-6.31	100.02	105.70
1	2A	2689	U	P-O3'-C3'	6.29	127.25	119.70
54	1w	47	U	C6-N1-C1'	-6.29	112.40	121.20
32	1a	1229	A	N1-C6-N6	-6.24	114.86	118.60
40	1i	121	ARG	C-N-CA	6.21	137.22	121.70
1	1A	1063	G	N1-C6-O6	-6.20	116.18	119.90
55	2x	14	A	C5-C6-N1	-6.20	114.60	117.70
55	2x	22	G	N3-C4-N9	-6.20	122.28	126.00
32	2a	754	C	N1-C2-O2	6.20	122.62	118.90
1	1A	2629	A	P-O3'-C3'	6.19	127.13	119.70
1	1A	2129	C	N1-C2-O2	6.17	122.60	118.90
32	2a	1279	A	OP1-P-O3'	6.17	118.76	105.20
1	1A	793	A	O5'-P-OP2	-6.15	100.17	105.70
1	2A	512	G	O4'-C1'-N9	6.10	113.08	108.20
55	1x	14	A	N1-C6-N6	6.09	122.26	118.60
1	1A	2848	G	O4'-C1'-N9	6.09	113.07	108.20
1	1A	805	G	N9-C4-C5	-6.03	102.99	105.40
1	1A	1082	U	N3-C4-C5	6.03	118.22	114.60
1	1A	784	A	O4'-C1'-N9	6.02	113.02	108.20
32	1a	1002	G	N3-C4-C5	-6.02	125.59	128.60
1	2A	277	C	C2-N1-C1'	6.02	125.42	118.80
54	1w	47	U	N3-C2-O2	-6.01	117.99	122.20
1	2A	2136	C	N1-C2-O2	5.99	122.50	118.90
1	1A	761	A	C8-N9-C4	5.99	108.20	105.80
1	1A	2616	C	C6-N1-C2	-5.99	117.91	120.30
1	1A	2553	G	N3-C4-N9	5.97	129.58	126.00
1	2A	277	C	N1-C2-O2	5.97	122.48	118.90
1	1A	2574	G	O5'-P-OP1	-5.96	100.33	105.70
32	2a	754	C	C2-N1-C1'	5.96	125.36	118.80
55	2x	22	G	C6-C5-N7	5.95	133.97	130.40
1	2A	2318	G	C4-N9-C1'	5.95	134.23	126.50
56	1y	56	C	C2-N3-C4	5.93	122.86	119.90
56	1y	33	U	C2-N1-C1'	5.89	124.77	117.70
1	2A	1204	A	O4'-C1'-N9	5.88	112.91	108.20
1	2A	1313	U	C2-N1-C1'	5.88	124.76	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1082	U	N3-C4-O4	-5.84	115.31	119.40
32	1a	1229	A	C5-C6-N6	5.83	128.37	123.70
1	1A	1380	G	C8-N9-C4	5.83	108.73	106.40
1	1A	2507	C	C6-N1-C2	-5.81	117.97	120.30
55	1x	46	G	N9-C4-C5	5.80	107.72	105.40
55	1x	14	A	C4-N9-C1'	5.77	136.69	126.30
32	1a	1002	G	C4-N9-C1'	5.77	134.00	126.50
55	1x	14	A	C8-N9-C1'	-5.75	117.35	127.70
1	1A	1296	G	O5'-P-OP2	-5.75	100.53	105.70
32	1a	90	U	N3-C2-O2	-5.75	118.18	122.20
32	1a	1002	G	N3-C4-N9	5.75	129.45	126.00
1	1A	2329	G	C5-C6-O6	-5.73	125.16	128.60
55	2x	22	G	C5-N7-C8	-5.71	101.44	104.30
1	1A	383	U	O4'-C1'-N1	5.70	112.76	108.20
54	2w	10	G	C4-N9-C1'	5.70	133.91	126.50
55	1x	46	G	N1-C2-N3	5.70	127.32	123.90
1	2A	90	U	N3-C2-O2	-5.69	118.22	122.20
32	2a	1272	G	N3-C4-N9	5.68	129.41	126.00
1	1A	2167	U	N3-C2-O2	-5.68	118.23	122.20
1	2A	228	A	OP1-P-O3'	5.66	117.65	105.20
1	1A	2621	A	C8-N9-C4	5.65	108.06	105.80
32	1a	841	U	C6-N1-C2	-5.65	117.61	121.00
1	2A	2153	G	C5-C6-O6	-5.65	125.21	128.60
1	1A	1009	A	N1-C6-N6	5.64	121.98	118.60
32	1a	1030(B)	C	C6-N1-C1'	-5.63	114.04	120.80
55	1x	22	G	C8-N9-C1'	5.62	134.31	127.00
32	1a	1065	U	P-O3'-C3'	5.62	126.45	119.70
1	1A	574	C	O5'-P-OP1	-5.62	100.64	105.70
55	2x	22	G	C8-N9-C1'	5.62	134.31	127.00
32	2a	1065	U	P-O3'-C3'	5.62	126.44	119.70
32	2a	79	G	C5-C6-O6	5.61	131.96	128.60
32	2a	1272	G	C2-N3-C4	-5.59	109.10	111.90
1	2A	614	U	N3-C2-O2	-5.58	118.29	122.20
1	1A	948	G	O5'-P-OP1	-5.58	100.68	105.70
1	1A	1075	C	N3-C2-O2	-5.58	118.00	121.90
1	2A	228	A	P-O3'-C3'	5.57	126.39	119.70
1	1A	2067	G	C8-N9-C4	-5.57	104.17	106.40
1	1A	2689	U	P-O3'-C3'	5.56	126.37	119.70
1	2A	1992	G	P-O3'-C3'	5.54	126.35	119.70
56	1y	70	G	N3-C4-N9	5.54	129.32	126.00
32	2a	1272	G	N9-C4-C5	-5.53	103.19	105.40
1	1A	845	G	O4'-C1'-N9	5.52	112.62	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1279	A	C8-N9-C4	-5.52	103.59	105.80
55	2x	46	G	C5-C6-N1	5.52	114.26	111.50
1	1A	1176	G	OP1-P-O3'	5.50	117.30	105.20
1	1A	1187	G	N1-C6-O6	-5.50	116.60	119.90
55	1x	22	G	C5-C6-N1	5.50	114.25	111.50
1	1A	1082	U	C2-N3-C4	-5.49	123.70	127.00
55	2x	46	G	N1-C2-N3	5.49	127.19	123.90
11	1P	43	GLY	C-N-CA	5.49	133.83	122.30
32	2a	1032	G	C6-N1-C2	5.48	128.39	125.10
1	1A	614	U	C2-N1-C1'	5.47	124.27	117.70
55	1x	46	G	C5-C6-N1	5.46	114.23	111.50
32	2a	841	U	C2-N1-C1'	5.46	124.25	117.70
55	1x	22	G	N7-C8-N9	5.46	115.83	113.10
1	1A	746	A	O4'-C1'-N9	5.45	112.56	108.20
1	2A	2123	G	C4-N9-C1'	-5.45	119.42	126.50
1	2A	847	U	C2-N1-C1'	5.44	124.23	117.70
32	1a	1027	C	C6-N1-C1'	5.44	127.33	120.80
1	1A	748	G	C4-N9-C1'	-5.43	119.44	126.50
1	1A	975	C	C2-N1-C1'	-5.43	112.83	118.80
1	1A	2096	U	N1-C2-O2	5.43	126.60	122.80
1	2A	528	A	P-O3'-C3'	5.43	126.21	119.70
1	2A	2155	G	C6-N1-C2	5.43	128.35	125.10
6	2G	139	LEU	CA-CB-CG	5.42	127.78	115.30
32	1a	1531	A	N7-C8-N9	5.42	116.51	113.80
56	1y	15	G	N3-C2-N2	5.39	123.67	119.90
1	1A	1372	U	C5-C4-O4	-5.39	122.67	125.90
1	1A	1572	A	O5'-P-OP2	-5.38	100.86	105.70
1	1A	1131	G	O4'-C1'-N9	5.37	112.50	108.20
1	1A	2501	C	C5-C6-N1	-5.37	118.32	121.00
32	1a	1030(B)	C	C5-C6-N1	5.36	123.68	121.00
56	1y	33	U	N1-C2-O2	5.36	126.55	122.80
56	1y	33	U	N3-C2-O2	-5.35	118.45	122.20
32	1a	1067	A	P-O3'-C3'	5.34	126.11	119.70
1	1A	1313	U	N3-C2-O2	-5.34	118.46	122.20
1	1A	1174	A	OP1-P-O3'	5.34	116.95	105.20
1	1A	774	A	C8-N9-C4	-5.33	103.67	105.80
1	2A	2422	A	O4'-C1'-N9	5.33	112.46	108.20
1	1A	983	A	C8-N9-C4	5.32	107.93	105.80
32	2a	266	G	N3-C4-C5	-5.32	125.94	128.60
1	2A	9	U	C5-C6-N1	5.32	125.36	122.70
32	2a	1263	C	C6-N1-C1'	-5.32	114.42	120.80
32	1a	913	A	P-O3'-C3'	5.31	126.08	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2167	U	N1-C2-O2	5.31	126.52	122.80
1	2A	1313	U	N3-C2-O2	-5.31	118.48	122.20
32	2a	266	G	P-O3'-C3'	5.29	126.06	119.70
1	1A	761	A	N7-C8-N9	-5.28	111.16	113.80
55	1x	56	C	N1-C2-O2	5.28	122.06	118.90
56	1y	56	C	N1-C2-O2	5.27	122.06	118.90
1	1A	2689	U	N3-C2-O2	-5.26	118.52	122.20
32	2a	913	A	P-O3'-C3'	5.26	126.01	119.70
32	1a	749	C	N1-C2-O2	5.26	122.05	118.90
1	1A	1785	A	C8-N9-C4	-5.25	103.70	105.80
55	1x	46	G	C5-C6-O6	-5.25	125.45	128.60
54	2w	11	C	C5-C6-N1	5.25	123.62	121.00
1	1A	1695	G	N3-C4-N9	5.23	129.14	126.00
56	2y	4	C	C2-N3-C4	5.23	122.52	119.90
1	1A	1075	C	C5-C4-N4	5.22	123.86	120.20
32	2a	1279	A	N7-C8-N9	5.21	116.41	113.80
1	1A	614	U	O4'-C1'-N1	5.20	112.36	108.20
1	1A	1644	C	C6-N1-C1'	-5.20	114.56	120.80
32	1a	1027	C	C2-N1-C1'	-5.20	113.08	118.80
32	1a	1331	G	O4'-C1'-N9	5.18	112.35	108.20
32	1a	90	U	N1-C2-O2	5.18	126.43	122.80
55	2x	46	G	N9-C4-C5	5.18	107.47	105.40
1	1A	2078	C	N1-C2-O2	5.17	122.00	118.90
1	2A	897	C	C5-C6-N1	5.17	123.58	121.00
32	2a	1029	C	N3-C2-O2	-5.17	118.28	121.90
32	2a	687	A	P-O3'-C3'	5.17	125.90	119.70
1	1A	2155	G	C2-N3-C4	5.16	114.48	111.90
1	2A	2490	G	N1-C6-O6	5.16	122.99	119.90
1	1A	748	G	C8-N9-C1'	5.14	133.69	127.00
1	1A	819	A	O5'-P-OP1	-5.14	101.07	105.70
34	2c	43	LEU	CA-CB-CG	5.14	127.11	115.30
32	2a	1263	C	C5-C4-N4	5.13	123.79	120.20
32	1a	1034	G	N1-C6-O6	-5.12	116.83	119.90
55	2x	14	A	C4-N9-C1'	5.12	135.52	126.30
56	1y	64	A	C5-C6-N6	5.12	127.79	123.70
1	2A	2123	G	C8-N9-C1'	5.12	133.65	127.00
56	1y	48	C	N1-C2-O2	-5.11	115.84	118.90
1	1A	1174	A	P-O3'-C3'	5.11	125.83	119.70
1	1A	1817	G	N1-C6-O6	-5.10	116.84	119.90
55	2x	46	G	C4-C5-N7	-5.10	108.76	110.80
1	2A	2689	U	N3-C2-O2	-5.09	118.64	122.20
32	1a	365	U	C2-N1-C1'	5.09	123.80	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1279	A	P-O3'-C3'	5.08	125.80	119.70
1	2A	2153	G	N1-C6-O6	5.08	122.95	119.90
9	1N	77	GLY	C-N-CA	5.07	134.38	121.70
1	2A	528	A	OP1-P-O3'	5.07	116.35	105.20
1	1A	12	U	C2-N1-C1'	5.07	123.78	117.70
32	1a	115	G	P-O3'-C3'	5.07	125.78	119.70
1	2A	1558	A	C2-N3-C4	-5.07	108.07	110.60
1	1A	1272	A	O5'-P-OP1	5.06	116.77	110.70
1	1A	881	G	N7-C8-N9	5.04	115.62	113.10
55	2x	46	G	N3-C4-C5	-5.04	126.08	128.60
1	1A	2553	G	N3-C4-C5	-5.03	126.08	128.60
55	1x	22	G	N3-C4-C5	5.01	131.11	128.60
1	1A	1063	G	N1-C2-N2	-5.01	111.69	116.20
1	2A	1395	A	O4'-C1'-N9	5.00	112.20	108.20

There are no chirality outliers.

There are no planarity outliers.

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%)	254 (93%)	19 (7%)	0	100	100
3	2D	273/276 (99%)	256 (94%)	17 (6%)	0	100	100
4	1E	202/206 (98%)	184 (91%)	17 (8%)	1 (0%)	29	48
4	2E	202/206 (98%)	187 (93%)	13 (6%)	2 (1%)	15	28
5	1F	201/210 (96%)	195 (97%)	5 (2%)	1 (0%)	29	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	2F	201/210 (96%)	177 (88%)	22 (11%)	2 (1%)	15	28
6	1G	179/182 (98%)	163 (91%)	15 (8%)	1 (1%)	25	43
6	2G	179/182 (98%)	156 (87%)	17 (10%)	6 (3%)	3	5
7	1H	172/180 (96%)	157 (91%)	14 (8%)	1 (1%)	25	43
7	2H	172/180 (96%)	153 (89%)	17 (10%)	2 (1%)	13	24
8	1I	144/148 (97%)	127 (88%)	16 (11%)	1 (1%)	22	39
8	2I	144/148 (97%)	116 (81%)	23 (16%)	5 (4%)	3	4
9	1N	138/140 (99%)	130 (94%)	8 (6%)	0	100	100
9	2N	138/140 (99%)	126 (91%)	11 (8%)	1 (1%)	22	39
10	1O	120/122 (98%)	110 (92%)	10 (8%)	0	100	100
10	2O	120/122 (98%)	109 (91%)	10 (8%)	1 (1%)	19	35
11	1P	147/150 (98%)	130 (88%)	14 (10%)	3 (2%)	7	12
11	2P	147/150 (98%)	129 (88%)	15 (10%)	3 (2%)	7	12
12	1Q	139/141 (99%)	127 (91%)	12 (9%)	0	100	100
12	2Q	139/141 (99%)	123 (88%)	16 (12%)	0	100	100
13	1R	116/118 (98%)	108 (93%)	7 (6%)	1 (1%)	17	31
13	2R	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
14	1S	108/112 (96%)	105 (97%)	3 (3%)	0	100	100
14	2S	108/112 (96%)	101 (94%)	6 (6%)	1 (1%)	17	31
15	1T	129/146 (88%)	119 (92%)	8 (6%)	2 (2%)	9	17
15	2T	129/146 (88%)	120 (93%)	9 (7%)	0	100	100
16	1U	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
16	2U	114/118 (97%)	109 (96%)	5 (4%)	0	100	100
17	1V	99/101 (98%)	91 (92%)	6 (6%)	2 (2%)	7	12
17	2V	99/101 (98%)	93 (94%)	5 (5%)	1 (1%)	15	28
18	1W	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
18	2W	110/113 (97%)	107 (97%)	3 (3%)	0	100	100
19	1X	93/96 (97%)	89 (96%)	2 (2%)	2 (2%)	6	10
19	2X	93/96 (97%)	85 (91%)	7 (8%)	1 (1%)	14	26
20	1Y	105/110 (96%)	99 (94%)	4 (4%)	2 (2%)	8	13
20	2Y	105/110 (96%)	98 (93%)	7 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	1Z	148/206 (72%)	130 (88%)	14 (10%)	4 (3%)	5	7
21	2Z	156/206 (76%)	128 (82%)	25 (16%)	3 (2%)	8	13
22	10	81/85 (95%)	78 (96%)	3 (4%)	0	100	100
22	20	81/85 (95%)	77 (95%)	3 (4%)	1 (1%)	13	24
23	11	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	14	26
23	21	95/98 (97%)	91 (96%)	3 (3%)	1 (1%)	14	26
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
25	13	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
25	23	57/60 (95%)	54 (95%)	2 (4%)	1 (2%)	8	14
26	14	67/71 (94%)	51 (76%)	11 (16%)	5 (8%)	1	1
26	24	67/71 (94%)	43 (64%)	20 (30%)	4 (6%)	1	1
27	15	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	25	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
28	16	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
28	26	51/54 (94%)	47 (92%)	4 (8%)	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%)	61 (98%)	1 (2%)	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	35 (100%)	0	0	100	100
33	1b	229/256 (90%)	193 (84%)	27 (12%)	9 (4%)	3	4
33	2b	229/256 (90%)	184 (80%)	35 (15%)	10 (4%)	2	3
34	1c	204/239 (85%)	188 (92%)	13 (6%)	3 (2%)	10	18
34	2c	204/239 (85%)	177 (87%)	24 (12%)	3 (2%)	10	18
35	1d	206/209 (99%)	193 (94%)	10 (5%)	3 (2%)	10	18
35	2d	206/209 (99%)	182 (88%)	19 (9%)	5 (2%)	6	9
36	1e	146/162 (90%)	134 (92%)	10 (7%)	2 (1%)	11	20
36	2e	146/162 (90%)	130 (89%)	15 (10%)	1 (1%)	22	39
37	1f	98/101 (97%)	89 (91%)	9 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	2f	98/101 (97%)	92 (94%)	6 (6%)	0	100	100
38	1g	153/156 (98%)	137 (90%)	14 (9%)	2 (1%)	12	21
38	2g	153/156 (98%)	134 (88%)	15 (10%)	4 (3%)	5	8
39	1h	135/138 (98%)	128 (95%)	7 (5%)	0	100	100
39	2h	135/138 (98%)	124 (92%)	11 (8%)	0	100	100
40	1i	125/128 (98%)	106 (85%)	19 (15%)	0	100	100
40	2i	125/128 (98%)	104 (83%)	19 (15%)	2 (2%)	9	17
41	1j	95/105 (90%)	81 (85%)	11 (12%)	3 (3%)	4	5
41	2j	94/105 (90%)	78 (83%)	14 (15%)	2 (2%)	7	11
42	1k	112/129 (87%)	98 (88%)	11 (10%)	3 (3%)	5	7
42	2k	112/129 (87%)	101 (90%)	9 (8%)	2 (2%)	8	14
43	1l	119/132 (90%)	112 (94%)	6 (5%)	1 (1%)	19	35
43	2l	119/132 (90%)	112 (94%)	6 (5%)	1 (1%)	19	35
44	1m	121/126 (96%)	107 (88%)	12 (10%)	2 (2%)	9	16
44	2m	120/126 (95%)	104 (87%)	14 (12%)	2 (2%)	9	16
45	1n	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
45	2n	58/61 (95%)	53 (91%)	5 (9%)	0	100	100
46	1o	86/89 (97%)	78 (91%)	5 (6%)	3 (4%)	3	4
46	2o	86/89 (97%)	80 (93%)	5 (6%)	1 (1%)	13	24
47	1p	80/88 (91%)	76 (95%)	4 (5%)	0	100	100
47	2p	80/88 (91%)	75 (94%)	5 (6%)	0	100	100
48	1q	97/105 (92%)	85 (88%)	10 (10%)	2 (2%)	7	11
48	2q	97/105 (92%)	86 (89%)	10 (10%)	1 (1%)	15	28
49	1r	66/88 (75%)	60 (91%)	6 (9%)	0	100	100
49	2r	66/88 (75%)	61 (92%)	4 (6%)	1 (2%)	10	18
50	1s	81/93 (87%)	71 (88%)	8 (10%)	2 (2%)	5	8
50	2s	81/93 (87%)	68 (84%)	11 (14%)	2 (2%)	5	8
51	1t	94/106 (89%)	83 (88%)	9 (10%)	2 (2%)	7	11
51	2t	94/106 (89%)	84 (89%)	9 (10%)	1 (1%)	14	26
52	1u	21/27 (78%)	21 (100%)	0	0	100	100
52	2u	21/27 (78%)	18 (86%)	3 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	11370/12128 (94%)	10332 (91%)	901 (8%)	137 (1%)	13	24

All (137) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	1P	38	GLN
21	1Z	53	ILE
26	14	53	GLU
33	1b	17	PHE
34	1c	66	VAL
44	1m	67	GLU
50	1s	27	GLU
50	1s	81	ARG
5	2F	130	ALA
6	2G	51	ARG
8	2I	40	THR
11	2P	45	LEU
33	2b	17	PHE
33	2b	74	LYS
38	2g	55	GLY
40	2i	56	LEU
50	2s	81	ARG
17	1V	100	ARG
20	1Y	78	ALA
21	1Z	52	SER
21	1Z	93	ASP
26	14	49	PHE
26	14	57	GLU
33	1b	8	LYS
33	1b	22	LYS
34	1c	65	ALA
35	1d	173	TRP
36	1e	85	GLY
41	1j	79	ARG
48	1q	68	ARG
51	1t	100	ILE
6	2G	42	GLY
6	2G	47	LYS
6	2G	96	ARG
7	2H	47	GLU
8	2I	10	GLU
11	2P	29	LYS

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Mol	Chain	Res	Type
19	2X	93	GLU
23	21	3	LYS
26	24	3	GLU
26	24	48	ARG
33	2b	126	GLU
33	2b	224	GLN
35	2d	3	ARG
38	2g	80	VAL
38	2g	153	HIS
40	2i	121	ARG
42	2k	49	GLY
44	2m	67	GLU
44	2m	106	ASN
48	2q	68	ARG
5	1F	130	ALA
11	1P	29	LYS
11	1P	36	LYS
17	1V	43	GLU
19	1X	2	LYS
26	14	62	ARG
33	1b	13	ALA
33	1b	126	GLU
36	1e	86	ALA
38	1g	52	GLU
42	1k	105	VAL
44	1m	46	LYS
46	1o	87	ILE
46	1o	88	ARG
48	1q	49	GLU
51	1t	10	LEU
8	2I	115	ALA
17	2V	79	VAL
21	2Z	93	ASP
21	2Z	146	ILE
22	20	13	GLY
33	2b	20	GLU
41	2j	79	ARG
4	1E	52	LEU
6	1G	43	LEU
15	1T	127	ALA
15	1T	128	GLU
33	1b	16	HIS

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Mol	Chain	Res	Type
33	1b	124	SER
33	1b	231	GLU
34	1c	71	ALA
41	1j	78	ASN
42	1k	77	MET
4	2E	52	LEU
5	2F	21	ALA
6	2G	43	LEU
7	2H	126	PRO
9	2N	2	LYS
10	2O	5	GLN
14	2S	84	GLN
33	2b	9	GLU
33	2b	123	ALA
33	2b	231	GLU
35	2d	107	ARG
35	2d	173	TRP
41	2j	78	ASN
43	2l	105	TYR
13	1R	107	ASP
23	1l	3	LYS
26	14	47	GLN
42	1k	49	GLY
43	1l	105	TYR
46	1o	19	PRO
8	2I	41	GLU
11	2P	44	GLY
25	23	59	VAL
34	2c	54	ARG
34	2c	107	GLN
35	2d	5	ILE
46	2o	87	ILE
50	2s	7	LYS
51	2t	47	GLY
8	1I	10	GLU
41	1j	77	PRO
8	2I	81	VAL
33	2b	16	HIS
34	2c	64	VAL
38	2g	152	ALA
20	1Y	55	TYR
21	1Z	157	LEU

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Mol	Chain	Res	Type
35	1d	88	VAL
38	1g	80	VAL
4	2E	71	GLY
19	1X	94	GLY
6	2G	159	VAL
26	24	11	PRO
26	24	45	GLY
33	2b	72	GLY
49	2r	27	GLY
35	1d	178	VAL
42	2k	105	VAL
7	1H	126	PRO
36	2e	69	VAL
21	2Z	171	ILE
35	2d	136	PRO
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%)	198 (92%)	17 (8%)	12	24
3	2D	215/218 (99%)	197 (92%)	18 (8%)	11	21
4	1E	164/166 (99%)	154 (94%)	10 (6%)	18	36
4	2E	164/166 (99%)	151 (92%)	13 (8%)	12	24
5	1F	160/166 (96%)	143 (89%)	17 (11%)	6	13
5	2F	159/166 (96%)	150 (94%)	9 (6%)	20	39
6	1G	143/156 (92%)	132 (92%)	11 (8%)	13	25
6	2G	143/156 (92%)	128 (90%)	15 (10%)	7	13
7	1H	144/148 (97%)	138 (96%)	6 (4%)	30	54
7	2H	144/148 (97%)	126 (88%)	18 (12%)	4	8
8	1I	113/124 (91%)	95 (84%)	18 (16%)	2	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	2I	105/124 (85%)	85 (81%)	20 (19%)	1	2
9	1N	118/119 (99%)	105 (89%)	13 (11%)	6	12
9	2N	118/119 (99%)	107 (91%)	11 (9%)	9	17
10	1O	100/100 (100%)	99 (99%)	1 (1%)	76	90
10	2O	100/100 (100%)	96 (96%)	4 (4%)	31	56
11	1P	115/116 (99%)	106 (92%)	9 (8%)	12	24
11	2P	115/116 (99%)	108 (94%)	7 (6%)	18	36
12	1Q	111/111 (100%)	104 (94%)	7 (6%)	18	34
12	2Q	111/111 (100%)	107 (96%)	4 (4%)	35	61
13	1R	101/101 (100%)	95 (94%)	6 (6%)	19	37
13	2R	101/101 (100%)	93 (92%)	8 (8%)	12	24
14	1S	86/88 (98%)	78 (91%)	8 (9%)	9	17
14	2S	85/88 (97%)	78 (92%)	7 (8%)	11	22
15	1T	115/127 (91%)	110 (96%)	5 (4%)	29	53
15	2T	113/127 (89%)	104 (92%)	9 (8%)	12	23
16	1U	93/94 (99%)	89 (96%)	4 (4%)	29	53
16	2U	93/94 (99%)	86 (92%)	7 (8%)	13	26
17	1V	80/82 (98%)	75 (94%)	5 (6%)	18	34
17	2V	80/82 (98%)	66 (82%)	14 (18%)	2	3
18	1W	90/92 (98%)	86 (96%)	4 (4%)	28	52
18	2W	90/92 (98%)	83 (92%)	7 (8%)	12	24
19	1X	77/78 (99%)	75 (97%)	2 (3%)	46	72
19	2X	77/78 (99%)	76 (99%)	1 (1%)	69	87
20	1Y	85/91 (93%)	78 (92%)	7 (8%)	11	22
20	2Y	85/91 (93%)	72 (85%)	13 (15%)	2	5
21	1Z	135/179 (75%)	117 (87%)	18 (13%)	4	7
21	2Z	137/179 (76%)	115 (84%)	22 (16%)	2	4
22	10	65/67 (97%)	63 (97%)	2 (3%)	40	67
22	20	65/67 (97%)	63 (97%)	2 (3%)	40	67
23	11	80/83 (96%)	76 (95%)	4 (5%)	24	46
23	21	80/83 (96%)	77 (96%)	3 (4%)	33	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	12	65/67 (97%)	64 (98%)	1 (2%)	65	85
24	22	65/67 (97%)	63 (97%)	2 (3%)	40	67
25	13	51/52 (98%)	46 (90%)	5 (10%)	8	15
25	23	50/52 (96%)	49 (98%)	1 (2%)	55	79
26	14	59/63 (94%)	54 (92%)	5 (8%)	10	21
26	24	53/63 (84%)	42 (79%)	11 (21%)	1	2
27	15	50/52 (96%)	48 (96%)	2 (4%)	31	56
27	25	50/52 (96%)	48 (96%)	2 (4%)	31	56
28	16	51/52 (98%)	45 (88%)	6 (12%)	5	10
28	26	50/52 (96%)	43 (86%)	7 (14%)	3	6
29	17	41/42 (98%)	38 (93%)	3 (7%)	14	27
29	27	41/42 (98%)	38 (93%)	3 (7%)	14	27
30	18	54/55 (98%)	50 (93%)	4 (7%)	13	27
30	28	54/55 (98%)	48 (89%)	6 (11%)	6	11
31	19	34/34 (100%)	33 (97%)	1 (3%)	42	69
31	29	34/34 (100%)	33 (97%)	1 (3%)	42	69
33	1b	192/220 (87%)	169 (88%)	23 (12%)	5	9
33	2b	187/220 (85%)	165 (88%)	22 (12%)	5	10
34	1c	142/188 (76%)	132 (93%)	10 (7%)	15	29
34	2c	140/188 (74%)	131 (94%)	9 (6%)	17	33
35	1d	169/181 (93%)	152 (90%)	17 (10%)	7	14
35	2d	173/181 (96%)	150 (87%)	23 (13%)	4	7
36	1e	113/123 (92%)	101 (89%)	12 (11%)	6	13
36	2e	114/123 (93%)	100 (88%)	14 (12%)	4	9
37	1f	84/90 (93%)	76 (90%)	8 (10%)	8	17
37	2f	85/90 (94%)	78 (92%)	7 (8%)	11	22
38	1g	119/127 (94%)	107 (90%)	12 (10%)	7	14
38	2g	120/127 (94%)	112 (93%)	8 (7%)	16	31
39	1h	114/119 (96%)	105 (92%)	9 (8%)	12	24
39	2h	114/119 (96%)	105 (92%)	9 (8%)	12	24
40	1i	90/99 (91%)	80 (89%)	10 (11%)	6	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	2i	89/99 (90%)	78 (88%)	11 (12%)	4	9
41	1j	66/92 (72%)	59 (89%)	7 (11%)	6	13
41	2j	69/92 (75%)	60 (87%)	9 (13%)	4	7
42	1k	82/99 (83%)	78 (95%)	4 (5%)	25	47
42	2k	83/99 (84%)	78 (94%)	5 (6%)	19	37
43	1l	96/108 (89%)	91 (95%)	5 (5%)	23	44
43	2l	96/108 (89%)	91 (95%)	5 (5%)	23	44
44	1m	93/101 (92%)	84 (90%)	9 (10%)	8	16
44	2m	92/101 (91%)	80 (87%)	12 (13%)	4	7
45	1n	49/50 (98%)	45 (92%)	4 (8%)	11	22
45	2n	49/50 (98%)	44 (90%)	5 (10%)	7	14
46	1o	78/80 (98%)	74 (95%)	4 (5%)	24	45
46	2o	78/80 (98%)	74 (95%)	4 (5%)	24	45
47	1p	69/74 (93%)	63 (91%)	6 (9%)	10	20
47	2p	68/74 (92%)	60 (88%)	8 (12%)	5	10
48	1q	94/97 (97%)	91 (97%)	3 (3%)	39	65
48	2q	94/97 (97%)	90 (96%)	4 (4%)	29	53
49	1r	59/77 (77%)	56 (95%)	3 (5%)	24	45
49	2r	59/77 (77%)	53 (90%)	6 (10%)	7	14
50	1s	69/80 (86%)	64 (93%)	5 (7%)	14	28
50	2s	67/80 (84%)	62 (92%)	5 (8%)	13	26
51	1t	70/82 (85%)	65 (93%)	5 (7%)	14	28
51	2t	70/82 (85%)	65 (93%)	5 (7%)	14	28
52	1u	18/22 (82%)	17 (94%)	1 (6%)	21	40
52	2u	18/22 (82%)	17 (94%)	1 (6%)	21	40
All	All	9303/10064 (92%)	8528 (92%)	775 (8%)	11	22

All (775) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	3	VAL
3	1D	16	MET
3	1D	22	SER

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Mol	Chain	Res	Type
3	1D	27	THR
3	1D	37	LEU
3	1D	38	LYS
3	1D	99	ASP
3	1D	116	GLN
3	1D	155	LEU
3	1D	162	SER
3	1D	181	GLU
3	1D	193	VAL
3	1D	221	VAL
3	1D	229	VAL
3	1D	242	ARG
3	1D	259	THR
3	1D	273	ARG
4	1E	12	THR
4	1E	21	VAL
4	1E	47	VAL
4	1E	59	VAL
4	1E	72	VAL
4	1E	75	VAL
4	1E	78	LEU
4	1E	97	LYS
4	1E	116	VAL
4	1E	181	LEU
5	1F	20	LEU
5	1F	24	LEU
5	1F	33	LEU
5	1F	57	VAL
5	1F	70	THR
5	1F	88	VAL
5	1F	106	ARG
5	1F	112	MET
5	1F	132	VAL
5	1F	140	LEU
5	1F	144	LYS
5	1F	157	VAL
5	1F	168	ARG
5	1F	183	VAL
5	1F	192	LEU
5	1F	195	ASP
5	1F	201	VAL
6	1G	5	VAL

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Mol	Chain	Res	Type
6	1G	7	LEU
6	1G	31	VAL
6	1G	43	LEU
6	1G	49	ASP
6	1G	91	ARG
6	1G	133	LEU
6	1G	140	ILE
6	1G	148	MET
6	1G	149	VAL
6	1G	159	VAL
7	1H	15	VAL
7	1H	16	SER
7	1H	23	ARG
7	1H	98	LEU
7	1H	113	VAL
7	1H	124	GLU
8	1I	10	GLU
8	1I	12	LEU
8	1I	15	VAL
8	1I	20	ASP
8	1I	40	THR
8	1I	45	LYS
8	1I	47	LEU
8	1I	50	ARG
8	1I	58	LEU
8	1I	77	LEU
8	1I	85	GLU
8	1I	87	LYS
8	1I	92	VAL
8	1I	101	LEU
8	1I	108	THR
8	1I	109	ILE
8	1I	133	HIS
8	1I	140	LEU
9	1N	1	MET
9	1N	14	VAL
9	1N	28	THR
9	1N	34	LEU
9	1N	46	VAL
9	1N	48	MET
9	1N	62	VAL
9	1N	67	LEU

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Mol	Chain	Res	Type
9	1N	68	GLU
9	1N	73	THR
9	1N	96	GLU
9	1N	137	LYS
9	1N	138	LEU
10	1O	116	SER
11	1P	45	LEU
11	1P	92	GLU
11	1P	95	VAL
11	1P	100	LEU
11	1P	102	ARG
11	1P	117	GLU
11	1P	133	SER
11	1P	147	LEU
11	1P	149	GLU
12	1Q	7	MET
12	1Q	16	ARG
12	1Q	75	THR
12	1Q	85	LYS
12	1Q	109	VAL
12	1Q	115	MET
12	1Q	133	ARG
13	1R	36	THR
13	1R	44	LEU
13	1R	67	LEU
13	1R	91	GLN
13	1R	100	LEU
13	1R	114	VAL
14	1S	3	ARG
14	1S	14	VAL
14	1S	15	ARG
14	1S	18	ILE
14	1S	25	ARG
14	1S	50	SER
14	1S	98	VAL
14	1S	110	LEU
15	1T	28	VAL
15	1T	39	ARG
15	1T	40	THR
15	1T	96	ARG
15	1T	128	GLU
16	1U	31	SER

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Mol	Chain	Res	Type
16	1U	74	LEU
16	1U	78	THR
16	1U	100	VAL
17	1V	28	GLU
17	1V	61	VAL
17	1V	73	SER
17	1V	82	ARG
17	1V	85	LYS
18	1W	11	ARG
18	1W	17	VAL
18	1W	60	ASN
18	1W	63	ASP
19	1X	60	ARG
19	1X	72	LYS
20	1Y	1	MET
20	1Y	7	VAL
20	1Y	70	SER
20	1Y	72	VAL
20	1Y	85	VAL
20	1Y	99	CYS
20	1Y	107	ASP
21	1Z	1	MET
21	1Z	8	TYR
21	1Z	31	ARG
21	1Z	33	LEU
21	1Z	46	LYS
21	1Z	52	SER
21	1Z	56	VAL
21	1Z	61	LEU
21	1Z	86	VAL
21	1Z	128	VAL
21	1Z	131	ARG
21	1Z	138	GLU
21	1Z	150	LEU
21	1Z	153	SER
21	1Z	154	ASP
21	1Z	155	LEU
21	1Z	165	VAL
21	1Z	171	ILE
22	10	14	ARG
22	10	55	ARG
23	11	46	LEU

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Mol	Chain	Res	Type
23	11	51	VAL
23	11	52	ARG
23	11	89	GLU
24	12	53	LEU
25	13	23	LEU
25	13	37	LEU
25	13	54	VAL
25	13	55	ARG
25	13	56	VAL
26	14	1	MET
26	14	49	PHE
26	14	52	THR
26	14	53	GLU
26	14	63	TYR
27	15	6	VAL
27	15	40	LYS
28	16	5	VAL
28	16	6	ARG
28	16	9	LEU
28	16	19	ARG
28	16	35	GLU
28	16	48	VAL
29	17	1	MET
29	17	43	THR
29	17	46	VAL
30	18	23	VAL
30	18	31	HIS
30	18	34	TRP
30	18	50	LEU
31	19	18	ARG
33	1b	8	LYS
33	1b	11	LEU
33	1b	12	GLU
33	1b	21	ARG
33	1b	24	TRP
33	1b	35	GLU
33	1b	37	ASN
33	1b	44	LEU
33	1b	54	THR
33	1b	60	ASP
33	1b	63	MET
33	1b	64	ARG

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Mol	Chain	Res	Type
33	1b	78	GLN
33	1b	82	ARG
33	1b	112	VAL
33	1b	121	LEU
33	1b	126	GLU
33	1b	127	ILE
33	1b	133	LYS
33	1b	144	ARG
33	1b	196	LEU
33	1b	208	ILE
33	1b	223	ILE
34	1c	3	ASN
34	1c	20	SER
34	1c	77	ILE
34	1c	82	GLU
34	1c	85	ARG
34	1c	89	GLU
34	1c	178	LEU
34	1c	182	ILE
34	1c	190	ARG
34	1c	196	LEU
35	1d	3	ARG
35	1d	49	ARG
35	1d	70	ILE
35	1d	77	ASN
35	1d	93	PHE
35	1d	100	ARG
35	1d	122	ARG
35	1d	135	LEU
35	1d	140	VAL
35	1d	152	SER
35	1d	157	LEU
35	1d	175	SER
35	1d	177	ASP
35	1d	178	VAL
35	1d	188	LEU
35	1d	194	LEU
35	1d	200	GLU
36	1e	10	MET
36	1e	20	GLN
36	1e	31	LEU
36	1e	40	ARG

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Mol	Chain	Res	Type
36	1e	41	VAL
36	1e	53	LEU
36	1e	63	ARG
36	1e	64	ARG
36	1e	79	GLU
36	1e	80	ILE
36	1e	82	VAL
36	1e	91	LEU
37	1f	10	LEU
37	1f	36	ARG
37	1f	45	LEU
37	1f	55	ASP
37	1f	70	ASP
37	1f	72	VAL
37	1f	75	LEU
37	1f	78	GLU
38	1g	32	ARG
38	1g	50	ILE
38	1g	59	LEU
38	1g	61	VAL
38	1g	66	VAL
38	1g	78	ARG
38	1g	90	GLU
38	1g	98	SER
38	1g	104	LEU
38	1g	113	GLU
38	1g	114	ARG
38	1g	115	ARG
39	1h	19	VAL
39	1h	39	LEU
39	1h	52	ASP
39	1h	92	ARG
39	1h	99	GLU
39	1h	112	LEU
39	1h	115	SER
39	1h	122	ARG
39	1h	133	LEU
40	1i	14	VAL
40	1i	25	LYS
40	1i	38	GLN
40	1i	64	THR
40	1i	87	GLN

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Mol	Chain	Res	Type
40	1i	96	LEU
40	1i	97	LYS
40	1i	103	THR
40	1i	121	ARG
40	1i	128	ARG
41	1j	35	SER
41	1j	46	ARG
41	1j	55	LYS
41	1j	81	THR
41	1j	92	THR
41	1j	98	ILE
41	1j	100	THR
42	1k	48	ILE
42	1k	87	THR
42	1k	104	GLN
42	1k	114	VAL
43	1l	13	LYS
43	1l	33	ARG
43	1l	36	VAL
43	1l	62	SER
43	1l	78	GLN
44	1m	3	ARG
44	1m	4	ILE
44	1m	14	ARG
44	1m	19	LEU
44	1m	49	THR
44	1m	64	TRP
44	1m	67	GLU
44	1m	70	LEU
44	1m	86	CYS
45	1n	3	ARG
45	1n	18	VAL
45	1n	23	ARG
45	1n	56	VAL
46	1o	24	SER
46	1o	27	VAL
46	1o	39	LEU
46	1o	88	ARG
47	1p	20	VAL
47	1p	22	THR
47	1p	27	LYS
47	1p	45	THR

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Mol	Chain	Res	Type
47	1p	60	LEU
47	1p	62	VAL
48	1q	52	LYS
48	1q	53	LEU
48	1q	60	ILE
49	1r	31	LEU
49	1r	54	ARG
49	1r	84	LYS
50	1s	6	LYS
50	1s	32	LYS
50	1s	37	ARG
50	1s	51	VAL
50	1s	71	LEU
51	1t	9	ASN
51	1t	10	LEU
51	1t	13	LEU
51	1t	24	LEU
51	1t	84	LEU
52	1u	6	ARG
3	2D	3	VAL
3	2D	34	VAL
3	2D	37	LEU
3	2D	38	LYS
3	2D	88	ARG
3	2D	113	VAL
3	2D	116	GLN
3	2D	126	GLN
3	2D	140	THR
3	2D	141	VAL
3	2D	142	VAL
3	2D	173	VAL
3	2D	193	VAL
3	2D	211	ARG
3	2D	221	VAL
3	2D	242	ARG
3	2D	259	THR
3	2D	267	SER
4	2E	7	VAL
4	2E	9	VAL
4	2E	12	THR
4	2E	21	VAL
4	2E	75	VAL

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Mol	Chain	Res	Type
4	2E	82	ARG
4	2E	90	THR
4	2E	116	VAL
4	2E	119	ARG
4	2E	145	LYS
4	2E	154	LYS
4	2E	181	LEU
4	2E	184	VAL
5	2F	20	LEU
5	2F	33	LEU
5	2F	106	ARG
5	2F	116	ASP
5	2F	145	GLU
5	2F	175	THR
5	2F	183	VAL
5	2F	192	LEU
5	2F	195	ASP
6	2G	3	LEU
6	2G	26	GLN
6	2G	28	VAL
6	2G	45	GLU
6	2G	51	ARG
6	2G	58	GLN
6	2G	60	LEU
6	2G	79	ASN
6	2G	91	ARG
6	2G	128	ARG
6	2G	133	LEU
6	2G	145	THR
6	2G	148	MET
6	2G	150	ASP
6	2G	173	LEU
7	2H	3	ARG
7	2H	4	ILE
7	2H	6	ARG
7	2H	7	LEU
7	2H	16	SER
7	2H	43	VAL
7	2H	49	VAL
7	2H	57	ASP
7	2H	71	LEU
7	2H	76	VAL

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Mol	Chain	Res	Type
7	2H	80	SER
7	2H	85	LYS
7	2H	88	LEU
7	2H	115	VAL
7	2H	124	GLU
7	2H	125	VAL
7	2H	129	THR
7	2H	130	ARG
8	2I	12	LEU
8	2I	25	TYR
8	2I	38	LEU
8	2I	58	LEU
8	2I	61	ARG
8	2I	66	GLU
8	2I	69	LYS
8	2I	77	LEU
8	2I	81	VAL
8	2I	82	ARG
8	2I	85	GLU
8	2I	87	LYS
8	2I	92	VAL
8	2I	96	ASP
8	2I	116	LEU
8	2I	117	GLU
8	2I	123	LEU
8	2I	126	TYR
8	2I	127	VAL
8	2I	144	VAL
9	2N	1	MET
9	2N	14	VAL
9	2N	15	LEU
9	2N	34	LEU
9	2N	38	HIS
9	2N	48	MET
9	2N	55	VAL
9	2N	62	VAL
9	2N	67	LEU
9	2N	68	GLU
9	2N	131	GLN
10	2O	14	THR
10	2O	78	ARG
10	2O	98	VAL

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Mol	Chain	Res	Type
10	2O	116	SER
11	2P	6	LEU
11	2P	7	ARG
11	2P	15	ARG
11	2P	45	LEU
11	2P	95	VAL
11	2P	125	VAL
11	2P	147	LEU
12	2Q	75	THR
12	2Q	109	VAL
12	2Q	110	THR
12	2Q	115	MET
13	2R	6	SER
13	2R	15	SER
13	2R	24	GLN
13	2R	44	LEU
13	2R	95	THR
13	2R	100	LEU
13	2R	111	LEU
13	2R	114	VAL
14	2S	23	ARG
14	2S	43	GLU
14	2S	50	SER
14	2S	58	LEU
14	2S	63	THR
14	2S	83	LYS
14	2S	110	LEU
15	2T	28	VAL
15	2T	39	ARG
15	2T	49	VAL
15	2T	50	ILE
15	2T	89	VAL
15	2T	95	ARG
15	2T	96	ARG
15	2T	104	ASN
15	2T	107	ASP
16	2U	5	LYS
16	2U	8	VAL
16	2U	55	ARG
16	2U	60	LEU
16	2U	74	LEU
16	2U	95	LEU

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Mol	Chain	Res	Type
16	2U	111	GLU
17	2V	7	THR
17	2V	28	GLU
17	2V	32	THR
17	2V	33	VAL
17	2V	38	LEU
17	2V	46	VAL
17	2V	52	VAL
17	2V	56	SER
17	2V	61	VAL
17	2V	66	ARG
17	2V	79	VAL
17	2V	85	LYS
17	2V	98	GLU
17	2V	99	ILE
18	2W	11	ARG
18	2W	17	VAL
18	2W	63	ASP
18	2W	67	ASP
18	2W	78	GLU
18	2W	92	ARG
18	2W	96	ILE
19	2X	82	GLN
20	2Y	1	MET
20	2Y	2	ARG
20	2Y	6	HIS
20	2Y	11	ASP
20	2Y	14	LEU
20	2Y	37	VAL
20	2Y	49	VAL
20	2Y	72	VAL
20	2Y	88	LYS
20	2Y	91	GLU
20	2Y	97	ARG
20	2Y	99	CYS
20	2Y	107	ASP
21	2Z	5	LEU
21	2Z	31	ARG
21	2Z	42	VAL
21	2Z	66	SER
21	2Z	67	LEU
21	2Z	71	VAL

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Mol	Chain	Res	Type
21	2Z	91	LEU
21	2Z	96	VAL
21	2Z	100	VAL
21	2Z	121	HIS
21	2Z	122	ARG
21	2Z	123	ASP
21	2Z	124	ILE
21	2Z	126	VAL
21	2Z	136	PHE
21	2Z	144	LEU
21	2Z	154	ASP
21	2Z	155	LEU
21	2Z	157	LEU
21	2Z	170	THR
21	2Z	171	ILE
21	2Z	174	VAL
22	20	14	ARG
22	20	55	ARG
23	21	17	SER
23	21	59	THR
23	21	65	SER
24	22	4	SER
24	22	59	ARG
25	23	59	VAL
26	24	15	ILE
26	24	27	THR
26	24	33	VAL
26	24	34	GLU
26	24	37	SER
26	24	49	PHE
26	24	58	ARG
26	24	59	PHE
26	24	63	TYR
26	24	67	TYR
26	24	68	ARG
27	25	40	LYS
27	25	55	ARG
28	26	5	VAL
28	26	6	ARG
28	26	9	LEU
28	26	14	THR
28	26	28	ARG

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Mol	Chain	Res	Type
28	26	32	ASN
28	26	45	LYS
29	27	1	MET
29	27	24	THR
29	27	46	VAL
30	28	3	LYS
30	28	4	MET
30	28	31	HIS
30	28	34	TRP
30	28	46	ARG
30	28	50	LEU
31	29	17	ILE
33	2b	9	GLU
33	2b	16	HIS
33	2b	24	TRP
33	2b	67	THR
33	2b	71	VAL
33	2b	76	GLN
33	2b	79	ASP
33	2b	80	ILE
33	2b	94	ASN
33	2b	107	THR
33	2b	112	VAL
33	2b	115	LEU
33	2b	118	LEU
33	2b	127	ILE
33	2b	142	LEU
33	2b	164	VAL
33	2b	168	THR
33	2b	185	ILE
33	2b	189	ASP
33	2b	226	ARG
33	2b	230	VAL
33	2b	236	TYR
34	2c	30	ARG
34	2c	43	LEU
34	2c	46	GLU
34	2c	47	LEU
34	2c	49	SER
34	2c	57	ILE
34	2c	69	HIS
34	2c	91	LEU

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Mol	Chain	Res	Type
34	2c	190	ARG
35	2d	47	ARG
35	2d	52	SER
35	2d	78	LEU
35	2d	81	GLU
35	2d	86	LYS
35	2d	91	SER
35	2d	112	VAL
35	2d	118	ARG
35	2d	127	THR
35	2d	135	LEU
35	2d	150	GLU
35	2d	155	LEU
35	2d	156	GLU
35	2d	157	LEU
35	2d	158	ILE
35	2d	168	ARG
35	2d	175	SER
35	2d	186	LEU
35	2d	188	LEU
35	2d	190	ASP
35	2d	193	ASP
35	2d	200	GLU
35	2d	209	ARG
36	2e	9	LYS
36	2e	13	ILE
36	2e	16	THR
36	2e	20	GLN
36	2e	31	LEU
36	2e	41	VAL
36	2e	51	VAL
36	2e	64	ARG
36	2e	66	MET
36	2e	72	GLN
36	2e	115	VAL
36	2e	116	THR
36	2e	144	THR
36	2e	149	GLU
37	2f	15	ASP
37	2f	21	LEU
37	2f	63	TYR
37	2f	69	GLU

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Mol	Chain	Res	Type
37	2f	83	ASP
37	2f	92	LYS
37	2f	94	GLN
38	2g	4	ARG
38	2g	15	ASP
38	2g	24	THR
38	2g	45	ASP
38	2g	53	LYS
38	2g	75	VAL
38	2g	79	ARG
38	2g	115	ARG
39	2h	26	VAL
39	2h	51	VAL
39	2h	52	ASP
39	2h	54	ASP
39	2h	95	VAL
39	2h	99	GLU
39	2h	112	LEU
39	2h	119	LEU
39	2h	129	VAL
40	2i	12	GLU
40	2i	14	VAL
40	2i	27	THR
40	2i	51	ARG
40	2i	64	THR
40	2i	65	VAL
40	2i	66	ARG
40	2i	89	ASN
40	2i	102	LEU
40	2i	111	ARG
40	2i	113	LYS
41	2j	8	LEU
41	2j	9	ARG
41	2j	19	SER
41	2j	38	ILE
41	2j	51	ARG
41	2j	67	THR
41	2j	72	VAL
41	2j	89	ASP
41	2j	100	THR
42	2k	14	VAL
42	2k	41	THR

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Mol	Chain	Res	Type
42	2k	87	THR
42	2k	105	VAL
42	2k	117	ASN
43	2l	13	LYS
43	2l	33	ARG
43	2l	62	SER
43	2l	83	VAL
43	2l	89	ARG
44	2m	19	LEU
44	2m	22	ILE
44	2m	32	GLU
44	2m	34	LEU
44	2m	47	ASP
44	2m	73	GLU
44	2m	80	ARG
44	2m	91	ARG
44	2m	102	ARG
44	2m	103	THR
44	2m	106	ASN
44	2m	108	ARG
45	2n	3	ARG
45	2n	6	LEU
45	2n	18	VAL
45	2n	23	ARG
45	2n	33	VAL
46	2o	22	THR
46	2o	39	LEU
46	2o	87	ILE
46	2o	88	ARG
47	2p	11	SER
47	2p	21	VAL
47	2p	33	ILE
47	2p	42	ARG
47	2p	60	LEU
47	2p	61	SER
47	2p	67	THR
47	2p	76	GLN
48	2q	14	LYS
48	2q	50	LYS
48	2q	55	ASP
48	2q	72	ARG
49	2r	31	LEU

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Mol	Chain	Res	Type
49	2r	45	SER
49	2r	46	GLU
49	2r	47	THR
49	2r	82	THR
49	2r	84	LYS
50	2s	12	ASP
50	2s	27	GLU
50	2s	37	ARG
50	2s	39	THR
50	2s	45	VAL
51	2t	15	ARG
51	2t	19	SER
51	2t	23	ARG
51	2t	31	SER
51	2t	41	ILE
52	2u	6	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (107) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	126	GLN
4	1E	48	GLN
4	1E	121	ASN
4	1E	180	ASN
5	1F	69	HIS
9	1N	8	GLN
11	1P	27	HIS
12	1Q	12	GLN
13	1R	13	HIS
13	1R	31	HIS
14	1S	68	GLN
16	1U	81	HIS
16	1U	94	ASN
19	1X	31	HIS
19	1X	82	GLN
20	1Y	6	HIS
21	1Z	34	ASN
21	1Z	73	GLN
21	1Z	151	HIS
23	11	56	GLN
24	12	9	GLN
25	13	32	GLN

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Mol	Chain	Res	Type
26	14	40	HIS
33	1b	16	HIS
33	1b	40	HIS
34	1c	6	HIS
34	1c	139	GLN
34	1c	162	GLN
34	1c	176	HIS
35	1d	116	GLN
35	1d	119	GLN
35	1d	123	HIS
35	1d	125	HIS
36	1e	20	GLN
36	1e	78	HIS
37	1f	13	ASN
37	1f	57	GLN
37	1f	73	ASN
37	1f	100	ASN
38	1g	13	GLN
38	1g	28	ASN
38	1g	86	GLN
40	1i	31	GLN
40	1i	89	ASN
40	1i	124	GLN
41	1j	56	HIS
43	1l	99	HIS
44	1m	12	ASN
44	1m	92	HIS
46	1o	9	GLN
50	1s	47	HIS
50	1s	83	HIS
3	2D	116	GLN
5	2F	69	HIS
5	2F	204	ASN
6	2G	26	GLN
6	2G	132	ASN
8	2I	133	HIS
9	2N	8	GLN
10	2O	3	GLN
11	2P	27	HIS
12	2Q	12	GLN
12	2Q	57	HIS
13	2R	71	GLN

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Mol	Chain	Res	Type
14	2S	38	GLN
14	2S	84	GLN
14	2S	95	HIS
15	2T	58	ASN
21	2Z	55	HIS
21	2Z	151	HIS
23	21	56	GLN
25	23	32	GLN
26	24	46	GLN
31	29	20	HIS
33	2b	76	GLN
33	2b	94	ASN
33	2b	135	GLN
33	2b	140	HIS
33	2b	224	GLN
34	2c	98	ASN
34	2c	162	GLN
35	2d	42	GLN
35	2d	77	ASN
35	2d	116	GLN
35	2d	119	GLN
35	2d	123	HIS
35	2d	125	HIS
37	2f	73	ASN
38	2g	86	GLN
40	2i	3	GLN
40	2i	58	HIS
40	2i	89	ASN
40	2i	117	HIS
41	2j	13	HIS
41	2j	21	GLN
41	2j	33	GLN
41	2j	62	HIS
42	2k	22	HIS
42	2k	117	ASN
44	2m	62	ASN
44	2m	77	ASN
45	2n	49	HIS
50	2s	23	ASN
50	2s	47	HIS
50	2s	69	HIS
50	2s	83	HIS

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Mol	Chain	Res	Type
51	2t	75	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2861/2915 (98%)	440 (15%)	30 (1%)
1	2A	2788/2915 (95%)	473 (16%)	23 (0%)
2	1B	119/121 (98%)	10 (8%)	0
2	2B	118/121 (97%)	21 (17%)	0
32	1a	1494/1521 (98%)	242 (16%)	0
32	2a	1498/1521 (98%)	283 (18%)	0
53	1v	12/24 (50%)	1 (8%)	0
53	2v	12/24 (50%)	1 (8%)	0
54	1w	70/76 (92%)	25 (35%)	0
54	2w	67/76 (88%)	18 (26%)	0
55	1x	74/77 (96%)	11 (14%)	0
55	2x	74/77 (96%)	10 (13%)	0
56	1y	71/76 (93%)	35 (49%)	0
56	2y	69/76 (90%)	22 (31%)	0
All	All	9327/9620 (96%)	1592 (17%)	53 (0%)

All (1592) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	10	G
1	1A	12	U
1	1A	13	A
1	1A	15	G
1	1A	27	G
1	1A	34	C
1	1A	35	G
1	1A	36	G
1	1A	38	A
1	1A	45	C
1	1A	55	G
1	1A	58	G
1	1A	63	U
1	1A	71	A
1	1A	72	U
1	1A	74	A
1	1A	75	G

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Mol	Chain	Res	Type
1	1A	84	A
1	1A	92	A
1	1A	118	A
1	1A	119	A
1	1A	120	U
1	1A	125	G
1	1A	154(A)	C
1	1A	181	A
1	1A	182	A
1	1A	196	A
1	1A	205	G
1	1A	215	G
1	1A	216	A
1	1A	222	A
1	1A	225	A
1	1A	228	A
1	1A	229	A
1	1A	233	A
1	1A	248	G
1	1A	266	G
1	1A	269	U
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(B)	G
1	1A	275	G
1	1A	279	C
1	1A	283	A
1	1A	311	A
1	1A	329	G
1	1A	330	A
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	386	G
1	1A	396	G

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Mol	Chain	Res	Type
1	1A	405	U
1	1A	411	G
1	1A	422	A
1	1A	428	A
1	1A	437	G
1	1A	444	C
1	1A	448	U
1	1A	451	C
1	1A	454	A
1	1A	456	C
1	1A	457	A
1	1A	481	G
1	1A	504	U
1	1A	505	A
1	1A	508	G
1	1A	509	C
1	1A	530	G
1	1A	531	C
1	1A	532	A
1	1A	533	G
1	1A	545	G
1	1A	549	G
1	1A	563	G
1	1A	573	G
1	1A	574	C
1	1A	575	A
1	1A	586	A
1	1A	592	G
1	1A	594	U
1	1A	603	A
1	1A	604	G
1	1A	607	U
1	1A	614(B)	G
1	1A	615	G
1	1A	627	A
1	1A	634	C
1	1A	637	A
1	1A	645	C
1	1A	646	A
1	1A	652(E)	G
1	1A	652(F)	G
1	1A	652(T)	C

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Mol	Chain	Res	Type
1	1A	669	G
1	1A	686	G
1	1A	730	C
1	1A	762	U
1	1A	765	G
1	1A	775	G
1	1A	776	G
1	1A	782	A
1	1A	784	A
1	1A	785	G
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	890	A
1	1A	892	G
1	1A	894	C
1	1A	896	A
1	1A	897	C
1	1A	898	C
1	1A	900	A
1	1A	910	A
1	1A	914	C
1	1A	932	G
1	1A	945	A
1	1A	946	G
1	1A	953	A
1	1A	959	A

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Mol	Chain	Res	Type
1	1A	961	C
1	1A	974	G
1	1A	975	C
1	1A	976	C
1	1A	983	A
1	1A	996	A
1	1A	1012	U
1	1A	1013	C
1	1A	1022	G
1	1A	1025	G
1	1A	1026	U
1	1A	1033	U
1	1A	1034	G
1	1A	1038	C
1	1A	1040	C
1	1A	1044	G
1	1A	1046	A
1	1A	1047	G
1	1A	1048	A
1	1A	1054	A
1	1A	1055	G
1	1A	1058	G
1	1A	1059	G
1	1A	1063	G
1	1A	1069	A
1	1A	1071	G
1	1A	1073	A
1	1A	1074	G
1	1A	1075	C
1	1A	1076	C
1	1A	1078	U
1	1A	1079	C
1	1A	1081	U
1	1A	1083	U
1	1A	1087	G
1	1A	1088	A
1	1A	1090	U
1	1A	1091	G
1	1A	1093	G
1	1A	1094	U
1	1A	1096	A
1	1A	1099	G

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Mol	Chain	Res	Type
1	1A	1101	U
1	1A	1102	C
1	1A	1111	A
1	1A	1112	G
1	1A	1115	G
1	1A	1116	C
1	1A	1118	C
1	1A	1128	A
1	1A	1135	C
1	1A	1136	G
1	1A	1142	U
1	1A	1155	A
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	1253	A
1	1A	1256	G
1	1A	1271	G
1	1A	1272	A
1	1A	1273	U
1	1A	1300	U
1	1A	1301	A
1	1A	1303	G
1	1A	1313	U
1	1A	1345	C
1	1A	1352	U
1	1A	1359	A
1	1A	1360	A
1	1A	1365	A
1	1A	1380	G
1	1A	1384	A
1	1A	1385	G
1	1A	1395	A
1	1A	1396	U
1	1A	1416	G
1	1A	1417	C
1	1A	1420	U

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Mol	Chain	Res	Type
1	1A	1421	G
1	1A	1428	C
1	1A	1445	A
1	1A	1450	G
1	1A	1455	G
1	1A	1467	C
1	1A	1468	C
1	1A	1482	G
1	1A	1493	C
1	1A	1494	A
1	1A	1500	G
1	1A	1508	A
1	1A	1509	C
1	1A	1509(A)	A
1	1A	1539	G
1	1A	1540	U
1	1A	1543	C
1	1A	1558	A
1	1A	1559	G
1	1A	1566	A
1	1A	1569	A
1	1A	1578	U
1	1A	1581	G
1	1A	1584	C
1	1A	1586	A
1	1A	1608	A
1	1A	1610	A
1	1A	1647	G
1	1A	1648	C
1	1A	1674	G
1	1A	1696	G
1	1A	1700	A
1	1A	1701	A
1	1A	1703	G
1	1A	1722	A
1	1A	1746	G
1	1A	1756	G
1	1A	1762	A
1	1A	1763	G
1	1A	1764	G
1	1A	1773	A
1	1A	1780	A

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Mol	Chain	Res	Type
1	1A	1782	C
1	1A	1791	A
1	1A	1800	C
1	1A	1801	G
1	1A	1816	G
1	1A	1828	G
1	1A	1829	A
1	1A	1847	A
1	1A	1861	G
1	1A	1877	A
1	1A	1878	G
1	1A	1900	A
1	1A	1906	G
1	1A	1927	A
1	1A	1929	G
1	1A	1930	G
1	1A	1937	A
1	1A	1938	A
1	1A	1941	C
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	1983	C
1	1A	1993	U
1	1A	1997	G
1	1A	2020	A
1	1A	2023	G
1	1A	2031	A
1	1A	2032	G
1	1A	2033	A
1	1A	2039	C
1	1A	2043	C
1	1A	2055	C
1	1A	2056	G
1	1A	2060	A
1	1A	2061	G
1	1A	2069	G
1	1A	2102	U
1	1A	2108	C

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Mol	Chain	Res	Type
1	1A	2110	G
1	1A	2113	U
1	1A	2116	G
1	1A	2118	U
1	1A	2120	G
1	1A	2121	G
1	1A	2127	G
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	2141	G
1	1A	2142	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	2161	C
1	1A	2162	G
1	1A	2165	G
1	1A	2166	G
1	1A	2171	A
1	1A	2172	U
1	1A	2173	A
1	1A	2181	G
1	1A	2182	G
1	1A	2183	C
1	1A	2184	G
1	1A	2189	U
1	1A	2192	G
1	1A	2198	A
1	1A	2206	G
1	1A	2207	G
1	1A	2208	A

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Mol	Chain	Res	Type
1	1A	2218	U
1	1A	2219	G
1	1A	2225	A
1	1A	2235	G
1	1A	2238	G
1	1A	2239	G
1	1A	2268	A
1	1A	2269	A
1	1A	2273	A
1	1A	2280	G
1	1A	2283	C
1	1A	2287	A
1	1A	2305	A
1	1A	2307	G
1	1A	2308	G
1	1A	2320	A
1	1A	2325	G
1	1A	2334	G
1	1A	2347	C
1	1A	2361	A
1	1A	2383	G
1	1A	2385	C
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	2435	A
1	1A	2439	A
1	1A	2441	C
1	1A	2448	A
1	1A	2449	U
1	1A	2468	G
1	1A	2476	A
1	1A	2478	A
1	1A	2491	U
1	1A	2502	G
1	1A	2505	G
1	1A	2518	A
1	1A	2529	G

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Mol	Chain	Res	Type
1	1A	2535	G
1	1A	2549	G
1	1A	2554	U
1	1A	2566	A
1	1A	2567	G
1	1A	2573	C
1	1A	2574	G
1	1A	2578	G
1	1A	2582	G
1	1A	2602	A
1	1A	2609	U
1	1A	2611	U
1	1A	2612	C
1	1A	2615	U
1	1A	2629	A
1	1A	2630	G
1	1A	2654	A
1	1A	2686	G
1	1A	2689	U
1	1A	2690	C
1	1A	2691	C
1	1A	2702	U
1	1A	2703	C
1	1A	2712(A)	A
1	1A	2713	A
1	1A	2714	G
1	1A	2726	U
1	1A	2733	A
1	1A	2758	A
1	1A	2765	A
1	1A	2766	G
1	1A	2778	A
1	1A	2790	A
1	1A	2791	C
1	1A	2792	G
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	2876	G

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Mol	Chain	Res	Type
1	1A	2892	A
1	1A	2894	G
1	1A	2895	U
2	1B	2	C
2	1B	15	A
2	1B	24	G
2	1B	56	G
2	1B	57	A
2	1B	65	C
2	1B	73	A
2	1B	85	G
2	1B	96	U
2	1B	110	G
32	1a	9	G
32	1a	31	G
32	1a	32	A
32	1a	39	G
32	1a	47	C
32	1a	48	C
32	1a	50	A
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	97	G
32	1a	98	G
32	1a	101	A
32	1a	116	A
32	1a	121	C
32	1a	131	C
32	1a	145	G
32	1a	147	G
32	1a	163	C
32	1a	174	C
32	1a	182	U
32	1a	189(F)	U
32	1a	189(J)	G
32	1a	195	A
32	1a	197	A
32	1a	202	U

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Mol	Chain	Res	Type
32	1a	203	U
32	1a	204	U
32	1a	216	G
32	1a	220	G
32	1a	247	G
32	1a	248	C
32	1a	251	G
32	1a	266	G
32	1a	267	C
32	1a	289	G
32	1a	318	G
32	1a	321	A
32	1a	328	C
32	1a	332	G
32	1a	344	A
32	1a	348	G
32	1a	351	G
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	367	U
32	1a	369	C
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	430	A
32	1a	439	A
32	1a	442	C
32	1a	452	A
32	1a	457	C
32	1a	461	A
32	1a	470	C
32	1a	474	G

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Mol	Chain	Res	Type
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	531	U
32	1a	532	A
32	1a	536	C
32	1a	547	A
32	1a	550	G
32	1a	559	A
32	1a	561	U
32	1a	562	C
32	1a	568	G
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	577	G
32	1a	596	C
32	1a	618	C
32	1a	630	G
32	1a	634	C
32	1a	653	A
32	1a	665	A
32	1a	666	G
32	1a	671	G
32	1a	687	A
32	1a	688	G
32	1a	695	A
32	1a	723	U
32	1a	724	G
32	1a	731	G
32	1a	734	G
32	1a	748	C
32	1a	749	C
32	1a	755	G
32	1a	766	A
32	1a	774	G
32	1a	777	A

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Mol	Chain	Res	Type
32	1a	792	A
32	1a	793	U
32	1a	794	A
32	1a	796	C
32	1a	817	C
32	1a	825	G
32	1a	827	U
32	1a	828	A
32	1a	840	C
32	1a	841	U
32	1a	851	G
32	1a	859	A
32	1a	864	A
32	1a	870	U
32	1a	887	G
32	1a	902	G
32	1a	914	A
32	1a	926	G
32	1a	927	G
32	1a	934	C
32	1a	935	A
32	1a	942	G
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	992	U
32	1a	993	G
32	1a	997	U
32	1a	1000	U
32	1a	1003	G
32	1a	1005	A
32	1a	1006	C
32	1a	1011	G
32	1a	1020	U
32	1a	1022	G

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Mol	Chain	Res	Type
32	1a	1023	G
32	1a	1025	U
32	1a	1026	G
32	1a	1027	C
32	1a	1028	C
32	1a	1029	C
32	1a	1030	C
32	1a	1030(A)	G
32	1a	1030(C)	G
32	1a	1031	G
32	1a	1039	C
32	1a	1044	A
32	1a	1054	C
32	1a	1063	C
32	1a	1065	U
32	1a	1066	C
32	1a	1068	G
32	1a	1081	G
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1123	A
32	1a	1124	G
32	1a	1125	U
32	1a	1127	G
32	1a	1132	C
32	1a	1134	G
32	1a	1137	C
32	1a	1138	G
32	1a	1139	G
32	1a	1146	A
32	1a	1152	A
32	1a	1158	C
32	1a	1159	U
32	1a	1182	G
32	1a	1183	A
32	1a	1184	G
32	1a	1187	G
32	1a	1196	U
32	1a	1197	G
32	1a	1201	A
32	1a	1202	G

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Mol	Chain	Res	Type
32	1a	1213	A
32	1a	1214	C
32	1a	1227	A
32	1a	1236	A
32	1a	1238	A
32	1a	1253	G
32	1a	1256	A
32	1a	1257	U
32	1a	1270	C
32	1a	1275	A
32	1a	1278	U
32	1a	1280	A
32	1a	1286	A
32	1a	1287	A
32	1a	1290	G
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1305	G
32	1a	1312	G
32	1a	1320	C
32	1a	1338	G
32	1a	1346	A
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1363(A)	A
32	1a	1379	G
32	1a	1397	C
32	1a	1419	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1446	U
32	1a	1447	A
32	1a	1456	G
32	1a	1492	A
32	1a	1494	G
32	1a	1499	A
32	1a	1503	A
32	1a	1504	G
32	1a	1506	U
32	1a	1517	G

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Mol	Chain	Res	Type
32	1a	1529	G
32	1a	1530	G
32	1a	1532	U
53	1v	13	A
54	1w	2	C
54	1w	3	C
54	1w	6	G
54	1w	8	4SU
54	1w	9	A
54	1w	14	A
54	1w	19	G
54	1w	20	U
54	1w	21	A
54	1w	23	A
54	1w	24	G
54	1w	25	C
54	1w	27	G
54	1w	46	7MG
54	1w	47	U
54	1w	48	C
54	1w	50	U
54	1w	60	U
54	1w	62	C
54	1w	66	U
54	1w	67	C
54	1w	68	C
54	1w	70	G
54	1w	73	A
54	1w	74	C
55	1x	9	G
55	1x	14	A
55	1x	16	C
55	1x	18	G
55	1x	19	G
55	1x	21	A
55	1x	47	U
55	1x	49	G
55	1x	61	C
55	1x	63	G
55	1x	69	C
56	1y	5	G
56	1y	6	G

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Mol	Chain	Res	Type
56	1y	8	4SU
56	1y	9	A
56	1y	11	C
56	1y	13	C
56	1y	14	A
56	1y	19	G
56	1y	20	U
56	1y	21	A
56	1y	26	A
56	1y	28	G
56	1y	29	G
56	1y	30	G
56	1y	35	A
56	1y	39	PSU
56	1y	40	C
56	1y	44	G
56	1y	45	U
56	1y	46	7MG
56	1y	47	U
56	1y	48	C
56	1y	49	C
56	1y	52	G
56	1y	53	G
56	1y	57	G
56	1y	58	A
56	1y	59	U
56	1y	61	C
56	1y	62	C
56	1y	65	G
56	1y	66	U
56	1y	69	G
56	1y	70	G
56	1y	71	G
1	2A	12	U
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	64	A

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Mol	Chain	Res	Type
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	157	U
1	2A	181	A
1	2A	196	A
1	2A	199	A
1	2A	205	G
1	2A	214	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	271(J)	C
1	2A	271(K)	U
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	271(O)	C
1	2A	272	G
1	2A	272(B)	G
1	2A	277	C
1	2A	278	A
1	2A	311	A
1	2A	317	G
1	2A	318	C
1	2A	327	G
1	2A	329	G
1	2A	330	A

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Mol	Chain	Res	Type
1	2A	333	G
1	2A	352	G
1	2A	354	G
1	2A	363	G
1	2A	363(B)	G
1	2A	363(D)	G
1	2A	386	G
1	2A	396	G
1	2A	399	G
1	2A	403	U
1	2A	411	G
1	2A	412	A
1	2A	421	U
1	2A	434	U
1	2A	443	A
1	2A	444	C
1	2A	454	A
1	2A	455	C
1	2A	456	C
1	2A	457	A
1	2A	480	A
1	2A	481	G
1	2A	494	G
1	2A	503	A
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	563	G
1	2A	568	U
1	2A	573	G
1	2A	574	C
1	2A	575	A
1	2A	583	G
1	2A	586	A
1	2A	595	C
1	2A	603	A

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Mol	Chain	Res	Type
1	2A	604	G
1	2A	607	U
1	2A	614(B)	G
1	2A	615	G
1	2A	627	A
1	2A	634	C
1	2A	637	A
1	2A	645	C
1	2A	652(B)	A
1	2A	652(C)	G
1	2A	669	G
1	2A	686	G
1	2A	717	G
1	2A	728	G
1	2A	730	C
1	2A	752	A
1	2A	753	C
1	2A	774	A
1	2A	775	G
1	2A	776	G
1	2A	782	A
1	2A	784	A
1	2A	785	G
1	2A	790	C
1	2A	792	G
1	2A	805	G
1	2A	812	C
1	2A	819	A
1	2A	825	C
1	2A	827	U
1	2A	857	C
1	2A	859	G
1	2A	874	G
1	2A	875	G
1	2A	877	U
1	2A	878	A
1	2A	879	G
1	2A	880	G
1	2A	884	C
1	2A	886	C
1	2A	887	A
1	2A	888	C

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Mol	Chain	Res	Type
1	2A	889	C
1	2A	893	C
1	2A	894	C
1	2A	895	U
1	2A	896	A
1	2A	900	A
1	2A	901	A
1	2A	904	C
1	2A	910	A
1	2A	914	C
1	2A	917	A
1	2A	932	G
1	2A	941	A
1	2A	945	A
1	2A	946	G
1	2A	952	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	1022	G
1	2A	1025	G
1	2A	1026	U
1	2A	1027	A
1	2A	1033	U
1	2A	1036	G
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	1126	A
1	2A	1128	A
1	2A	1129	A

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Mol	Chain	Res	Type
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1139	G
1	2A	1142(A)	A
1	2A	1144	G
1	2A	1148	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	1236	G
1	2A	1244	G
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A
1	2A	1273	U
1	2A	1287	A
1	2A	1300	U
1	2A	1301	A
1	2A	1303	G
1	2A	1314	C
1	2A	1321	A
1	2A	1352	U
1	2A	1359	A
1	2A	1360	A
1	2A	1365	A
1	2A	1368	G
1	2A	1370	C
1	2A	1373	A
1	2A	1379	A
1	2A	1384	A
1	2A	1385	G
1	2A	1386	C
1	2A	1410	G
1	2A	1412	A
1	2A	1416	G
1	2A	1417	C
1	2A	1420	U

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Mol	Chain	Res	Type
1	2A	1421	G
1	2A	1427	A
1	2A	1428	C
1	2A	1437	C
1	2A	1445	A
1	2A	1449	A
1	2A	1450	G
1	2A	1455	G
1	2A	1460	A
1	2A	1461	G
1	2A	1463	C
1	2A	1467	C
1	2A	1471	A
1	2A	1482	G
1	2A	1490	A
1	2A	1493	C
1	2A	1494	A
1	2A	1496	A
1	2A	1497	U
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1531	C
1	2A	1532	C
1	2A	1533	G
1	2A	1545	A
1	2A	1547	C
1	2A	1558	A
1	2A	1569	A
1	2A	1574	C
1	2A	1578	U
1	2A	1580	A
1	2A	1583	A
1	2A	1584	C
1	2A	1586	A
1	2A	1588	C
1	2A	1595	G
1	2A	1608	A
1	2A	1609	A
1	2A	1610	A
1	2A	1629	U
1	2A	1648	C

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Mol	Chain	Res	Type
1	2A	1653	G
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	1756	G
1	2A	1762	A
1	2A	1763	G
1	2A	1764	G
1	2A	1773	A
1	2A	1780	A
1	2A	1782	C
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1812	A
1	2A	1816	G
1	2A	1829	A
1	2A	1835	G
1	2A	1847	A
1	2A	1848	A
1	2A	1861	G
1	2A	1877	A
1	2A	1878	G
1	2A	1889	A
1	2A	1896	G
1	2A	1900	A
1	2A	1906	G
1	2A	1913	A
1	2A	1914	C
1	2A	1929	G
1	2A	1930	G
1	2A	1936	A
1	2A	1938	A
1	2A	1955	U
1	2A	1963	U

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Mol	Chain	Res	Type
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1993	U
1	2A	1997	G
1	2A	2020	A
1	2A	2023	G
1	2A	2031	A
1	2A	2033	A
1	2A	2035	G
1	2A	2036	C
1	2A	2043	C
1	2A	2044	C
1	2A	2055	C
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G
1	2A	2069	G
1	2A	2093	G
1	2A	2099	U
1	2A	2101	G
1	2A	2110	G
1	2A	2111	C
1	2A	2112	G
1	2A	2113	U
1	2A	2116	G
1	2A	2117	A
1	2A	2120	G
1	2A	2122	U
1	2A	2125	G
1	2A	2126	A
1	2A	2127	G
1	2A	2128	C
1	2A	2129	C
1	2A	2131	G
1	2A	2132	U
1	2A	2134	A
1	2A	2135	A
1	2A	2136	C
1	2A	2137	C
1	2A	2138	C

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Mol	Chain	Res	Type
1	2A	2139	C
1	2A	2141	G
1	2A	2145	C
1	2A	2146	C
1	2A	2150	U
1	2A	2151	G
1	2A	2153	G
1	2A	2154	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	2183	C
1	2A	2185	C
1	2A	2189	U
1	2A	2192	G
1	2A	2193	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	2267	A
1	2A	2275	C
1	2A	2278	A
1	2A	2280	G
1	2A	2283	C
1	2A	2287	A
1	2A	2288	A
1	2A	2298	A
1	2A	2305	A

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Mol	Chain	Res	Type
1	2A	2308	G
1	2A	2319	G
1	2A	2320	A
1	2A	2325	G
1	2A	2327	A
1	2A	2334	G
1	2A	2335	A
1	2A	2336	A
1	2A	2346	A
1	2A	2347	C
1	2A	2354	G
1	2A	2376	A
1	2A	2383	G
1	2A	2385	C
1	2A	2403	C
1	2A	2406	U
1	2A	2422	A
1	2A	2424	C
1	2A	2425	A
1	2A	2429	G
1	2A	2430	A
1	2A	2434	A
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2445	G
1	2A	2448	A
1	2A	2465	C
1	2A	2469	A
1	2A	2476	A
1	2A	2477	C
1	2A	2480	C
1	2A	2481	G
1	2A	2482	G
1	2A	2491	U
1	2A	2494	G
1	2A	2502	G
1	2A	2505	G
1	2A	2507	C
1	2A	2518	A
1	2A	2520	C
1	2A	2525	G

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Mol	Chain	Res	Type
1	2A	2529	G
1	2A	2554	U
1	2A	2557	G
1	2A	2566	A
1	2A	2567	G
1	2A	2573	C
1	2A	2582	G
1	2A	2585	U
1	2A	2602	A
1	2A	2611	U
1	2A	2612	C
1	2A	2630	G
1	2A	2634	G
1	2A	2654	A
1	2A	2689	U
1	2A	2690	C
1	2A	2702	U
1	2A	2703	C
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G
1	2A	2718	G
1	2A	2726	U
1	2A	2733	A
1	2A	2751	G
1	2A	2759	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
1	2A	2802	G
1	2A	2803	C
1	2A	2807	G
1	2A	2820	A
1	2A	2821	A
1	2A	2830	G
1	2A	2835	A
1	2A	2872	G
1	2A	2892	A

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Mol	Chain	Res	Type
1	2A	2894	G
1	2A	2897	U
2	2B	2	C
2	2B	8	U
2	2B	13	A
2	2B	17	C
2	2B	19	G
2	2B	33	G
2	2B	41	U
2	2B	42	C
2	2B	44	G
2	2B	56	G
2	2B	73	A
2	2B	74	U
2	2B	75	G
2	2B	85	G
2	2B	88	C
2	2B	89	G
2	2B	106	G
2	2B	108	U
2	2B	110	G
2	2B	117	G
2	2B	120	A
32	2a	7	G
32	2a	9	G
32	2a	22	G
32	2a	32	A
32	2a	39	G
32	2a	41	G
32	2a	47	C
32	2a	48	C
32	2a	50	A
32	2a	51	A
32	2a	66	G
32	2a	73	G
32	2a	88	A
32	2a	89	C
32	2a	101	A
32	2a	105	G
32	2a	116	A
32	2a	121	C
32	2a	131	C

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Mol	Chain	Res	Type
32	2a	142	G
32	2a	143	A
32	2a	144	G
32	2a	162	A
32	2a	163	C
32	2a	182	U
32	2a	189	G
32	2a	189(E)	U
32	2a	189(F)	U
32	2a	189(J)	G
32	2a	190	U
32	2a	195	A
32	2a	197	A
32	2a	201	C
32	2a	202	U
32	2a	204	U
32	2a	216	G
32	2a	217	C
32	2a	231	G
32	2a	247	G
32	2a	251	G
32	2a	258	G
32	2a	266	G
32	2a	267	C
32	2a	289	G
32	2a	316	G
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	345	C
32	2a	348	G
32	2a	350	G
32	2a	351	G
32	2a	352	C
32	2a	353	A
32	2a	354	G
32	2a	355	C
32	2a	367	U
32	2a	372	C
32	2a	384	G
32	2a	388	G
32	2a	389	A

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Mol	Chain	Res	Type
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	412	A
32	2a	413	G
32	2a	421	U
32	2a	423	G
32	2a	424	G
32	2a	429	U
32	2a	430	A
32	2a	441	A
32	2a	442	C
32	2a	452	A
32	2a	461	A
32	2a	470	C
32	2a	475	G
32	2a	484	G
32	2a	485	G
32	2a	496	A
32	2a	498	U
32	2a	505	G
32	2a	506	G
32	2a	509	A
32	2a	510	A
32	2a	511	C
32	2a	518	C
32	2a	527	7MG
32	2a	531	U
32	2a	532	A
32	2a	534	U
32	2a	547	A
32	2a	559	A
32	2a	562	C
32	2a	564	C
32	2a	568	G
32	2a	572	A
32	2a	573	A
32	2a	576	G
32	2a	577	G
32	2a	581	G
32	2a	596	C
32	2a	598	U

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Mol	Chain	Res	Type
32	2a	601	C
32	2a	614	A
32	2a	630	G
32	2a	653	A
32	2a	665	A
32	2a	671	G
32	2a	687	A
32	2a	688	G
32	2a	723	U
32	2a	731	G
32	2a	749	C
32	2a	755	G
32	2a	763	G
32	2a	773	G
32	2a	774	G
32	2a	777	A
32	2a	787	A
32	2a	793	U
32	2a	794	A
32	2a	812	C
32	2a	815	A
32	2a	817	C
32	2a	819	A
32	2a	821	G
32	2a	827	U
32	2a	828	A
32	2a	833	U
32	2a	840	C
32	2a	841	U
32	2a	851	G
32	2a	859	A
32	2a	887	G
32	2a	891	U
32	2a	902	G
32	2a	914	A
32	2a	926	G
32	2a	927	G
32	2a	934	C
32	2a	935	A
32	2a	958	A
32	2a	960	U
32	2a	961	U

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Mol	Chain	Res	Type
32	2a	968	A
32	2a	969	A
32	2a	971	G
32	2a	974	A
32	2a	975	A
32	2a	976	G
32	2a	977	A
32	2a	992	U
32	2a	993	G
32	2a	997	U
32	2a	998	G
32	2a	999	C
32	2a	1001	A
32	2a	1001(A)	G
32	2a	1002	G
32	2a	1003	G
32	2a	1004	A
32	2a	1005	A
32	2a	1006	C
32	2a	1009	G
32	2a	1011	G
32	2a	1019	C
32	2a	1020	U
32	2a	1021	G
32	2a	1022	G
32	2a	1023	G
32	2a	1025	U
32	2a	1027	C
32	2a	1028	C
32	2a	1029	C
32	2a	1030	C
32	2a	1030(A)	G
32	2a	1031	G
32	2a	1032	G
32	2a	1035	A
32	2a	1036	G
32	2a	1037	C
32	2a	1039	C
32	2a	1040	U
32	2a	1043	C
32	2a	1046	A
32	2a	1050	G

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Mol	Chain	Res	Type
32	2a	1051	C
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1077	G
32	2a	1081	G
32	2a	1086	U
32	2a	1093	A
32	2a	1094	G
32	2a	1095	U
32	2a	1097	C
32	2a	1101	A
32	2a	1105	A
32	2a	1118	C
32	2a	1129	C
32	2a	1130	A
32	2a	1133	G
32	2a	1136	U
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G
32	2a	1140	C
32	2a	1141	C
32	2a	1146	A
32	2a	1147	C
32	2a	1152	A
32	2a	1157	A
32	2a	1159	U
32	2a	1160	G
32	2a	1177	G
32	2a	1181	G
32	2a	1182	G
32	2a	1184	G
32	2a	1193	G
32	2a	1194	U
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	1236	A

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Mol	Chain	Res	Type
32	2a	1238	A
32	2a	1240	U
32	2a	1241	G
32	2a	1246	C
32	2a	1255	G
32	2a	1256	A
32	2a	1257	U
32	2a	1260	C
32	2a	1261	A
32	2a	1264	C
32	2a	1270	C
32	2a	1272	G
32	2a	1273	G
32	2a	1277	C
32	2a	1279	A
32	2a	1280	A
32	2a	1281	U
32	2a	1287	A
32	2a	1289	A
32	2a	1299	A
32	2a	1302	U
32	2a	1306	A
32	2a	1310	G
32	2a	1323	G
32	2a	1340	A
32	2a	1347	G
32	2a	1353	G
32	2a	1357	A
32	2a	1363	C
32	2a	1363(A)	A
32	2a	1364	U
32	2a	1368	G
32	2a	1370	G
32	2a	1382	C
32	2a	1383	C
32	2a	1397	C
32	2a	1398	A
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1447	A
32	2a	1456	G

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Mol	Chain	Res	Type
32	2a	1487	G
32	2a	1492	A
32	2a	1499	A
32	2a	1503	A
32	2a	1504	G
32	2a	1505	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
54	2w	3	C
54	2w	4	C
54	2w	5	G
54	2w	8	4SU
54	2w	13	C
54	2w	14	A
54	2w	19	G
54	2w	22	G
54	2w	46	7MG
54	2w	48	C
54	2w	62	C
54	2w	63	G
54	2w	65	G
54	2w	68	C
54	2w	69	G
54	2w	70	G
54	2w	73	A
54	2w	74	C
55	2x	5	G
55	2x	6	G
55	2x	9	G
55	2x	18	G
55	2x	21	A
55	2x	31	G
55	2x	47	U
55	2x	61	C
55	2x	63	G
55	2x	69	C
56	2y	15	G

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Mol	Chain	Res	Type
56	2y	19	G
56	2y	23	A
56	2y	25	C
56	2y	27	G
56	2y	45	U
56	2y	47	U
56	2y	49	C
56	2y	52	G
56	2y	53	G
56	2y	54	5MU
56	2y	55	PSU
56	2y	56	C
56	2y	57	G
56	2y	58	A
56	2y	59	U
56	2y	61	C
56	2y	65	G
56	2y	68	C
56	2y	69	G
56	2y	70	G
56	2y	73	A

All (53) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	196	A
1	1A	249	C
1	1A	266	G
1	1A	271(K)	U
1	1A	278	A
1	1A	548	A
1	1A	685	A
1	1A	746	A
1	1A	764	A
1	1A	774	A
1	1A	827	U
1	1A	895	U
1	1A	974	G
1	1A	1047	G
1	1A	1065	U
1	1A	1067	A
1	1A	1174	A

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Mol	Chain	Res	Type
1	1A	1176	G
1	1A	1379	A
1	1A	1442	G
1	1A	1508	A
1	1A	1992	G
1	1A	2134	A
1	1A	2181	G
1	1A	2183	C
1	1A	2406	U
1	1A	2422	A
1	1A	2430	A
1	1A	2629	A
1	1A	2689	U
1	2A	196	A
1	2A	228	A
1	2A	266	G
1	2A	271(M)	G
1	2A	277	C
1	2A	528	A
1	2A	752	A
1	2A	827	U
1	2A	856	C
1	2A	900	A
1	2A	1026	U
1	2A	1210	A
1	2A	1420	U
1	2A	1442	G
1	2A	1460	A
1	2A	1530	C
1	2A	1608	A
1	2A	1653	G
1	2A	1913	A
1	2A	1992	G
1	2A	2119	A
1	2A	2126	A
1	2A	2689	U

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	PSU	1y	32	56	17,21,22	1.47	2 (11%)	20,30,33	3.17	6 (30%)
55	4SU	2x	8	55	14,21,22	1.32	2 (14%)	15,30,33	2.41	2 (13%)
1	5MC	1A	1962	1	15,22,23	1.34	1 (6%)	19,32,35	1.23	1 (5%)
56	PSU	2y	32	56	17,21,22	1.37	2 (11%)	20,30,33	3.14	5 (25%)
56	PSU	1y	39	56	17,21,22	1.40	2 (11%)	20,30,33	3.09	6 (30%)
1	PSU	2A	1911	1	17,21,22	1.61	3 (17%)	20,30,33	3.17	6 (30%)
55	4SU	1x	8	55	14,21,22	1.37	2 (14%)	15,30,33	2.94	2 (13%)
1	OMG	1A	2251	1,55,57	18,26,27	1.34	2 (11%)	20,38,41	2.35	6 (30%)
32	2MG	2a	1207	32	19,26,27	1.27	2 (10%)	21,38,41	2.29	7 (33%)
32	5MC	1a	967	32	15,22,23	1.36	1 (6%)	19,32,35	1.21	2 (10%)
55	5MU	2x	54	55	15,22,23	1.03	1 (6%)	16,32,35	1.75	2 (12%)
32	5MC	1a	1407	32	15,22,23	1.34	1 (6%)	19,32,35	1.32	2 (10%)
32	UR3	2a	1498	32	14,22,23	0.77	1 (7%)	15,32,35	0.85	1 (6%)
55	PSU	2x	55	55	17,21,22	1.50	2 (11%)	20,30,33	3.17	6 (30%)
56	4SU	2y	8	56	14,21,22	1.25	1 (7%)	15,30,33	1.40	2 (13%)
1	5MC	2A	1942	1	15,22,23	1.40	1 (6%)	19,32,35	1.30	3 (15%)
55	31H	1x	76	55,57	28,34,35	1.07	3 (10%)	23,47,50	1.60	5 (21%)
1	4OC	2A	1920	1	15,22,24	0.68	0	17,31,35	1.44	1 (5%)
1	PSU	1A	2605	1,57	17,21,22	1.62	3 (17%)	20,30,33	3.11	6 (30%)
56	5MU	1y	54	56	15,22,23	1.03	1 (6%)	16,32,35	2.16	1 (6%)
32	2MG	1a	1207	32	19,26,27	1.32	2 (10%)	21,38,41	2.41	8 (38%)
32	7MG	1a	527	32	22,26,27	1.77	4 (18%)	28,39,42	2.72	8 (28%)
32	5MC	1a	1404	32	15,22,23	1.32	1 (6%)	19,32,35	1.37	3 (15%)
32	4OC	2a	1402	32,57	16,23,24	0.65	0	17,32,35	1.43	1 (5%)
54	PSU	2w	39	54	17,21,22	1.42	3 (17%)	20,30,33	2.78	6 (30%)
1	OMG	2A	2251	1,55,57	18,26,27	1.07	2 (11%)	20,38,41	1.98	5 (25%)
54	MIA	2w	37	54	20,27,32	1.75	3 (15%)	22,39,47	2.18	7 (31%)
32	4OC	1a	1402	32	16,23,24	0.53	0	17,32,35	1.22	1 (5%)
32	5MC	1a	1400	32	15,22,23	1.26	1 (6%)	19,32,35	1.45	2 (10%)
32	M2G	1a	966	32	20,27,28	1.42	3 (15%)	22,40,43	2.27	6 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	5MC	2a	1407	32	15,22,23	1.34	1 (6%)	19,32,35	1.31	3 (15%)
32	MA6	1a	1519	32	19,26,27	0.80	0	18,38,41	1.63	3 (16%)
54	PSU	2w	32	54	17,21,22	1.41	2 (11%)	20,30,33	3.33	6 (30%)
32	PSU	1a	516	32	17,21,22	1.59	3 (17%)	20,30,33	3.05	6 (30%)
32	5MC	2a	1404	32	15,22,23	1.35	1 (6%)	19,32,35	1.38	2 (10%)
54	F3N	1w	76	1,54	30,36,37	1.45	5 (16%)	29,51,54	1.24	1 (3%)
54	PSU	1w	32	54,57	17,21,22	1.50	2 (11%)	20,30,33	3.15	6 (30%)
54	5MU	1w	54	54	15,22,23	1.10	1 (6%)	16,32,35	1.94	2 (12%)
43	0TD	1l	92	43	4,9,10	3.07	1 (25%)	3,11,13	6.61	1 (33%)
43	0TD	2l	92	43	4,9,10	3.08	1 (25%)	3,11,13	6.12	1 (33%)
54	5MU	2w	54	54	15,22,23	1.06	2 (13%)	16,32,35	2.17	1 (6%)
32	M2G	2a	966	32	20,27,28	1.39	3 (15%)	22,40,43	2.06	5 (22%)
1	5MU	1A	1939	1,57	15,22,23	1.19	2 (13%)	16,32,35	1.81	2 (12%)
56	5MU	2y	54	56	15,22,23	1.04	1 (6%)	16,32,35	2.18	1 (6%)
1	2MU	1A	2552	1	14,22,24	0.88	1 (7%)	14,31,36	0.82	1 (7%)
32	MA6	2a	1519	32	19,26,27	0.83	0	18,38,41	1.61	2 (11%)
54	PSU	1w	39	54	17,21,22	1.51	2 (11%)	20,30,33	2.79	6 (30%)
32	UR3	1a	1498	32	14,22,23	0.86	1 (7%)	15,32,35	0.85	1 (6%)
54	4SU	2w	8	54	14,21,22	1.22	1 (7%)	15,30,33	1.33	2 (13%)
1	PSU	1A	1917	1	17,21,22	1.56	2 (11%)	20,30,33	3.07	6 (30%)
56	4SU	1y	8	56	14,21,22	1.24	1 (7%)	15,30,33	1.54	2 (13%)
32	7MG	2a	527	32,57	22,26,27	1.81	4 (18%)	28,39,42	2.68	10 (35%)
56	MIA	1y	37	56	18,24,32	1.14	2 (11%)	18,35,47	1.19	2 (11%)
1	5MC	1A	1942	1	15,22,23	1.25	1 (6%)	19,32,35	1.44	3 (15%)
54	PSU	1w	55	54	17,21,22	1.53	3 (17%)	20,30,33	3.20	6 (30%)
32	5MC	2a	967	32,57	15,22,23	1.30	1 (6%)	19,32,35	1.35	3 (15%)
56	PSU	1y	55	56	17,21,22	1.46	3 (17%)	20,30,33	3.14	6 (30%)
1	5MC	2A	1962	1,57	15,22,23	1.38	1 (6%)	19,32,35	1.34	3 (15%)
54	4SU	1w	8	54	14,21,22	1.31	2 (14%)	15,30,33	1.45	2 (13%)
1	5MU	1A	1915	1	15,22,23	0.98	2 (13%)	16,32,35	1.88	2 (12%)
55	5MC	2x	32	55	15,22,23	1.27	1 (6%)	19,32,35	1.48	4 (21%)
1	5MU	2A	1915	1,57	15,22,23	1.06	1 (6%)	16,32,35	1.92	1 (6%)
54	PSU	2w	55	54	17,21,22	1.38	2 (11%)	20,30,33	3.37	7 (35%)
1	PSU	2A	2605	1	17,21,22	1.67	3 (17%)	20,30,33	3.15	6 (30%)
1	2MA	1A	2503	1,57	17,25,26	1.23	1 (5%)	19,37,40	2.05	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	5MC	2a	1400	32	15,22,23	1.35	1 (6%)	19,32,35	1.29	3 (15%)
56	PSU	2y	39	56	17,21,22	1.46	2 (11%)	20,30,33	3.75	6 (30%)
56	MIA	2y	37	56	18,24,32	1.11	2 (11%)	18,35,47	1.37	3 (16%)
54	7MG	1w	46	54	22,26,27	1.73	4 (18%)	28,39,42	2.79	8 (28%)
55	31H	2x	76	55,57	28,34,35	1.10	3 (10%)	23,47,50	1.52	3 (13%)
1	5MU	2A	1939	1,57	15,22,23	1.11	2 (13%)	16,32,35	1.79	2 (12%)
32	MA6	2a	1518	32	19,26,27	0.84	0	18,38,41	1.42	2 (11%)
56	PSU	2y	55	56	17,21,22	1.43	2 (11%)	20,30,33	3.32	6 (30%)
54	MIA	1w	37	54	24,31,32	2.17	3 (12%)	26,44,47	2.78	10 (38%)
56	7MG	1y	46	56	22,26,27	1.86	4 (18%)	28,39,42	2.94	10 (35%)
1	2MU	2A	2552	1,57	14,22,24	0.86	0	14,31,36	0.71	1 (7%)
54	F3N	2w	76	1,54	30,36,37	1.41	5 (16%)	29,51,54	1.21	2 (6%)
1	4OC	1A	1920	1	15,22,24	0.76	0	17,31,35	1.35	2 (11%)
32	MA6	1a	1518	32	19,26,27	0.81	0	18,38,41	1.45	2 (11%)
1	PSU	2A	1917	1	17,21,22	1.62	3 (17%)	20,30,33	3.29	6 (30%)
55	PSU	1x	55	55	17,21,22	1.50	2 (11%)	20,30,33	3.19	6 (30%)
1	2MA	2A	2503	1,57	17,25,26	1.44	2 (11%)	19,37,40	1.95	3 (15%)
1	PSU	1A	1911	1	17,21,22	1.52	2 (11%)	20,30,33	2.94	5 (25%)
55	5MC	1x	32	55	15,22,23	1.29	1 (6%)	19,32,35	1.58	4 (21%)
54	7MG	2w	46	54	22,26,27	1.76	4 (18%)	28,39,42	2.75	9 (32%)
55	5MU	1x	54	55	15,22,23	1.15	1 (6%)	16,32,35	2.01	1 (6%)
56	7MG	2y	46	56	22,26,27	1.88	4 (18%)	28,39,42	2.95	12 (42%)
32	PSU	2a	516	32	17,21,22	1.48	3 (17%)	20,30,33	3.06	7 (35%)

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
56	PSU	1y	32	56	-	0/7/25/26	0/2/2/2
55	4SU	2x	8	55	-	0/5/25/26	0/2/2/2
1	5MC	1A	1962	1	-	2/5/25/26	0/2/2/2
56	PSU	2y	32	56	-	0/7/25/26	0/2/2/2
56	PSU	1y	39	56	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/5/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	1A	2251	1,55,57	-	0/5/27/28	0/3/3/3
32	2MG	2a	1207	32	-	0/5/27/28	0/3/3/3
32	5MC	1a	967	32	-	1/5/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/5/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/5/25/26	0/2/2/2
32	UR3	2a	1498	32	-	2/5/25/26	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
56	4SU	2y	8	56	-	0/5/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/5/25/26	0/2/2/2
55	31H	1x	76	55,57	-	3/18/40/41	0/3/3/3
1	4OC	2A	1920	1	-	0/7/27/30	0/2/2/2
1	PSU	1A	2605	1,57	-	0/7/25/26	0/2/2/2
56	5MU	1y	54	56	-	0/5/25/26	0/2/2/2
32	2MG	1a	1207	32	-	2/5/27/28	0/3/3/3
32	7MG	1a	527	32	-	2/7/37/38	0/3/3/3
32	5MC	1a	1404	32	-	0/5/25/26	0/2/2/2
32	4OC	2a	1402	32,57	-	3/9/29/30	0/2/2/2
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	1,55,57	-	1/5/27/28	0/3/3/3
54	MIA	2w	37	54	-	2/7/29/34	0/3/3/3
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
32	5MC	1a	1400	32	-	2/5/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
32	5MC	2a	1407	32	-	0/5/25/26	0/2/2/2
32	MA6	1a	1519	32	-	2/7/29/30	0/3/3/3
54	PSU	2w	32	54	-	1/7/25/26	0/2/2/2
32	PSU	1a	516	32	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/5/25/26	0/2/2/2
54	F3N	1w	76	1,54	-	0/15/37/38	0/4/4/4
54	PSU	1w	32	54,57	-	0/7/25/26	0/2/2/2
54	5MU	1w	54	54	-	0/5/25/26	0/2/2/2
43	0TD	1l	92	43	-	1/3/12/14	-
43	0TD	2l	92	43	-	2/3/12/14	-
54	5MU	2w	54	54	-	0/5/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
1	5MU	1A	1939	1,57	-	0/5/25/26	0/2/2/2
56	5MU	2y	54	56	-	2/5/25/26	0/2/2/2
1	2MU	1A	2552	1	-	0/7/27/28	0/2/2/2
32	MA6	2a	1519	32	-	3/7/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/5/25/26	0/2/2/2
54	4SU	2w	8	54	-	0/5/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
56	4SU	1y	8	56	-	3/5/25/26	0/2/2/2
32	7MG	2a	527	32,57	-	3/7/37/38	0/3/3/3
56	MIA	1y	37	56	-	2/3/25/34	0/3/3/3
1	5MC	1A	1942	1	-	0/5/25/26	0/2/2/2
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	32,57	-	0/5/25/26	0/2/2/2
56	PSU	1y	55	56	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	1,57	-	2/5/25/26	0/2/2/2
54	4SU	1w	8	54	-	0/5/25/26	0/2/2/2
1	5MU	1A	1915	1	-	0/5/25/26	0/2/2/2
55	5MC	2x	32	55	-	0/5/25/26	0/2/2/2
1	5MU	2A	1915	1,57	-	0/5/25/26	0/2/2/2
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
1	2MA	1A	2503	1,57	-	2/3/25/26	0/3/3/3
32	5MC	2a	1400	32	-	0/5/25/26	0/2/2/2
56	PSU	2y	39	56	-	0/7/25/26	0/2/2/2
56	MIA	2y	37	56	-	3/3/25/34	0/3/3/3
54	7MG	1w	46	54	-	3/7/37/38	0/3/3/3
55	31H	2x	76	55,57	-	3/18/40/41	0/3/3/3
1	5MU	2A	1939	1,57	-	0/5/25/26	0/2/2/2
32	MA6	2a	1518	32	-	0/7/29/30	0/3/3/3
56	PSU	2y	55	56	-	4/7/25/26	0/2/2/2
54	MIA	1w	37	54	-	3/11/33/34	0/3/3/3
56	7MG	1y	46	56	-	5/7/37/38	0/3/3/3
1	2MU	2A	2552	1,57	-	0/7/27/28	0/2/2/2
54	F3N	2w	76	1,54	-	0/15/37/38	0/4/4/4
1	4OC	1A	1920	1	-	1/7/27/30	0/2/2/2
32	MA6	1a	1518	32	-	0/7/29/30	0/3/3/3
1	PSU	2A	1917	1	-	2/7/25/26	0/2/2/2
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	1,57	-	1/3/25/26	0/3/3/3
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
55	5MC	1x	32	55	-	0/5/25/26	0/2/2/2
54	7MG	2w	46	54	-	0/7/37/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	5MU	1x	54	55	-	0/5/25/26	0/2/2/2
56	7MG	2y	46	56	-	3/7/37/38	0/3/3/3
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2

All (162) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	37	MIA	C13-C14	7.01	1.52	1.32
54	1w	37	MIA	C2-S10	-6.60	1.70	1.75
54	2w	37	MIA	C2-S10	-6.47	1.70	1.75
43	2l	92	0TD	CB-SB	-5.91	1.69	1.84
43	1l	92	0TD	CB-SB	-5.72	1.70	1.84
32	2a	527	7MG	C6-C5	5.49	1.49	1.41
1	2A	1942	5MC	C5-C4	5.02	1.49	1.41
56	2y	46	7MG	C6-C5	4.97	1.48	1.41
32	1a	967	5MC	C5-C4	4.95	1.49	1.41
56	2y	46	7MG	C5-C4	4.94	1.48	1.39
1	2A	1962	5MC	C5-C4	4.92	1.49	1.41
1	2A	2503	2MA	C6-C5	4.86	1.48	1.41
54	2w	46	7MG	C6-C5	4.86	1.48	1.41
56	1y	46	7MG	C5-C4	4.83	1.48	1.39
32	2a	1404	5MC	C5-C4	4.81	1.48	1.41
56	1y	46	7MG	C6-C5	4.81	1.48	1.41
32	1a	527	7MG	C6-C5	4.76	1.48	1.41
32	2a	1400	5MC	C5-C4	4.76	1.48	1.41
32	1a	1404	5MC	C5-C4	4.71	1.48	1.41
1	1A	1962	5MC	C5-C4	4.70	1.48	1.41
32	2a	967	5MC	C5-C4	4.66	1.48	1.41
32	1a	1407	5MC	C5-C4	4.64	1.48	1.41
1	2A	2605	PSU	C5-C1'	-4.63	1.48	1.52
32	2a	1407	5MC	C5-C4	4.62	1.48	1.41
1	2A	1911	PSU	C5-C1'	-4.60	1.48	1.52
1	1A	1942	5MC	C5-C4	4.56	1.48	1.41
1	1A	2605	PSU	C5-C1'	-4.53	1.48	1.52
55	2x	32	5MC	C5-C4	4.50	1.48	1.41
32	2a	1207	2MG	C6-C5	4.50	1.49	1.41
54	1w	46	7MG	C5-C4	4.50	1.48	1.39
32	1a	1207	2MG	C6-C5	4.48	1.49	1.41
55	1x	32	5MC	C5-C4	4.47	1.48	1.41
1	2A	1917	PSU	C5-C1'	-4.45	1.48	1.52
32	1a	1400	5MC	C5-C4	4.43	1.48	1.41
54	1w	76	F3N	CB-CG	-4.43	1.40	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1a	966	M2G	C6-C5	4.41	1.49	1.41
1	1A	2251	OMG	C6-C5	4.38	1.48	1.41
32	1a	527	7MG	C5-C4	4.36	1.47	1.39
54	1w	46	7MG	C6-C5	4.35	1.47	1.41
54	2w	46	7MG	C5-C4	4.34	1.47	1.39
32	2a	527	7MG	C5-C4	4.32	1.47	1.39
54	2w	76	F3N	CB-CG	-4.30	1.41	1.51
32	1a	516	PSU	C5-C1'	-4.24	1.48	1.52
1	1A	2503	2MA	C6-C5	4.16	1.47	1.41
1	1A	1917	PSU	C5-C1'	-4.13	1.48	1.52
54	1w	32	PSU	C5-C1'	-4.08	1.48	1.52
54	1w	8	4SU	C4-S4	-4.06	1.60	1.67
56	2y	8	4SU	C4-S4	-4.05	1.60	1.67
32	2a	966	M2G	C6-C5	4.00	1.48	1.41
55	2x	8	4SU	C4-S4	-4.00	1.60	1.67
56	1y	8	4SU	C4-S4	-3.95	1.60	1.67
54	1w	39	PSU	C5-C1'	-3.92	1.48	1.52
54	1w	55	PSU	C5-C1'	-3.87	1.48	1.52
56	1y	32	PSU	C5-C1'	-3.74	1.49	1.52
56	1y	39	PSU	C4-C5	3.74	1.49	1.41
55	2x	55	PSU	C5-C1'	-3.71	1.49	1.52
32	2a	516	PSU	C5-C1'	-3.70	1.49	1.52
54	2w	55	PSU	C4-C5	3.70	1.49	1.41
32	1a	527	7MG	C5-N7	-3.68	1.33	1.39
1	1A	1911	PSU	C5-C1'	-3.67	1.49	1.52
55	1x	54	5MU	C4-C5	3.65	1.49	1.41
54	2w	32	PSU	C4-C5	3.65	1.49	1.41
54	2w	8	4SU	C4-S4	-3.64	1.60	1.67
56	1y	32	PSU	C4-C5	3.63	1.49	1.41
56	2y	32	PSU	C4-C5	3.63	1.49	1.41
1	1A	1911	PSU	C4-C5	3.62	1.49	1.41
55	2x	55	PSU	C4-C5	3.59	1.49	1.41
54	1w	46	7MG	C5-N7	-3.58	1.33	1.39
55	1x	55	PSU	C4-C5	3.57	1.49	1.41
56	2y	55	PSU	C4-C5	3.51	1.49	1.41
54	2w	46	7MG	C5-N7	-3.50	1.33	1.39
54	2w	39	PSU	C5-C1'	-3.50	1.49	1.52
56	2y	39	PSU	C4-C5	3.49	1.48	1.41
56	1y	55	PSU	C5-C1'	-3.48	1.49	1.52
1	1A	1917	PSU	C4-C5	3.46	1.48	1.41
56	2y	39	PSU	C5-C1'	-3.45	1.49	1.52
54	1w	39	PSU	C4-C5	3.44	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	2251	OMG	C6-C5	3.43	1.47	1.41
56	1y	55	PSU	C4-C5	3.41	1.48	1.41
55	1x	55	PSU	C5-C1'	-3.41	1.49	1.52
56	1y	46	7MG	C5-N7	-3.41	1.34	1.39
55	1x	8	4SU	C2-N3	-3.38	1.31	1.38
55	1x	8	4SU	C4-S4	-3.38	1.61	1.67
56	1y	54	5MU	C4-C5	3.35	1.48	1.41
1	2A	2605	PSU	C4-C5	3.35	1.48	1.41
32	2a	516	PSU	C4-C5	3.35	1.48	1.41
56	2y	55	PSU	C5-C1'	-3.35	1.49	1.52
54	1w	76	F3N	O4'-C1'	3.34	1.45	1.41
56	2y	54	5MU	C4-C5	3.32	1.48	1.41
1	2A	1939	5MU	C4-C5	3.31	1.48	1.41
54	1w	54	5MU	C4-C5	3.30	1.48	1.41
54	2w	54	5MU	C4-C5	3.30	1.48	1.41
1	1A	1939	5MU	C4-C5	3.29	1.48	1.41
54	1w	55	PSU	C4-C5	3.29	1.48	1.41
32	2a	966	M2G	C2-N2	3.29	1.40	1.34
1	2A	1915	5MU	C4-C5	3.28	1.48	1.41
54	1w	32	PSU	C4-C5	3.28	1.48	1.41
1	2A	1917	PSU	C4-C5	3.27	1.48	1.41
32	1a	966	M2G	C2-N2	3.26	1.40	1.34
54	2w	39	PSU	C4-C5	3.24	1.48	1.41
1	1A	2605	PSU	C4-C5	3.24	1.48	1.41
32	1a	516	PSU	C4-C5	3.21	1.48	1.41
54	2w	76	F3N	O4'-C1'	3.17	1.45	1.41
56	2y	46	7MG	C5-N7	-3.16	1.34	1.39
55	2x	76	31H	C5-C4	-3.11	1.32	1.40
55	2x	54	5MU	C4-C5	3.11	1.48	1.41
54	2w	32	PSU	C5-C1'	-3.06	1.49	1.52
32	2a	527	7MG	C5-N7	-3.06	1.34	1.39
1	2A	1911	PSU	C4-C5	3.04	1.48	1.41
56	1y	39	PSU	C5-C1'	-2.97	1.49	1.52
1	1A	1915	5MU	C4-C5	2.88	1.47	1.41
54	1w	76	F3N	C5-C4	-2.84	1.33	1.40
56	1y	37	MIA	C2-N3	2.76	1.36	1.32
54	2w	37	MIA	C5-C4	2.76	1.48	1.40
56	1y	37	MIA	C5-C4	2.73	1.48	1.40
56	2y	37	MIA	C5-C4	2.73	1.48	1.40
54	2w	76	F3N	C5-C4	-2.72	1.33	1.40
54	2w	55	PSU	C5-C1'	-2.70	1.49	1.52
56	2y	32	PSU	C5-C1'	-2.67	1.50	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2a	966	M2G	C5-C4	2.64	1.47	1.40
32	1a	527	7MG	C4-N9	-2.63	1.33	1.38
56	2y	37	MIA	C2-N3	2.55	1.36	1.32
32	2a	1207	2MG	C5-C4	2.55	1.47	1.40
54	2w	76	F3N	C6-C5	-2.55	1.33	1.43
1	1A	1939	5MU	C2-N3	-2.52	1.33	1.38
55	2x	76	31H	C6-C5	-2.52	1.33	1.43
1	2A	2503	2MA	C5-C4	2.52	1.47	1.40
55	1x	76	31H	C5-N7	-2.51	1.30	1.39
32	2a	527	7MG	C4-N9	-2.51	1.33	1.38
55	2x	8	4SU	C2-N3	-2.47	1.33	1.38
55	1x	76	31H	C5-C4	-2.46	1.34	1.40
1	1A	2251	OMG	C5-C4	2.43	1.47	1.40
54	1w	46	7MG	C4-N9	-2.43	1.33	1.38
32	1a	966	M2G	C5-C4	2.42	1.47	1.40
55	1x	76	31H	C6-C5	-2.42	1.34	1.43
54	1w	37	MIA	C5-C4	2.41	1.47	1.40
32	1a	1207	2MG	C5-C4	2.38	1.47	1.40
54	2w	46	7MG	C4-N9	-2.37	1.33	1.38
32	1a	516	PSU	O4'-C1'	-2.36	1.41	1.44
54	2w	37	MIA	C2-N3	2.34	1.37	1.34
1	2A	2251	OMG	C5-C4	2.33	1.47	1.40
32	1a	1498	UR3	C4-N3	2.30	1.41	1.38
1	2A	2605	PSU	C2-N3	-2.29	1.33	1.38
54	1w	76	F3N	C6-C5	-2.26	1.34	1.43
54	2w	76	F3N	C5-N7	-2.22	1.31	1.39
1	1A	2605	PSU	O4'-C1'	-2.20	1.41	1.44
56	2y	46	7MG	C4-N3	2.18	1.37	1.34
54	1w	76	F3N	C5-N7	-2.18	1.31	1.39
32	2a	516	PSU	O4'-C1'	-2.15	1.41	1.44
56	1y	46	7MG	C4-N3	2.14	1.37	1.34
1	2A	1911	PSU	O4'-C1'	-2.14	1.41	1.44
1	2A	1917	PSU	C2-N3	-2.12	1.34	1.38
56	1y	55	PSU	O4'-C1'	-2.12	1.41	1.44
1	2A	1939	5MU	C2-N3	-2.10	1.34	1.38
54	2w	39	PSU	O4'-C1'	-2.09	1.41	1.44
32	2a	1498	UR3	C4-N3	2.07	1.41	1.38
55	2x	76	31H	C5-N7	-2.07	1.32	1.39
1	1A	1915	5MU	C2-N3	-2.06	1.34	1.38
1	1A	2552	2MU	C2-N3	-2.04	1.34	1.38
54	1w	55	PSU	C2-N1	-2.04	1.34	1.38
54	2w	54	5MU	C2-N3	-2.02	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	8	4SU	C2-N3	-2.01	1.34	1.38

All (349) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1l	92	0TD	CSB-SB-CB	11.32	124.11	101.85
43	2l	92	0TD	CSB-SB-CB	-10.51	81.18	101.85
56	2y	39	PSU	N1-C2-N3	-10.26	120.28	128.43
55	1x	8	4SU	C2-N3-C4	9.94	129.57	115.15
54	2w	32	PSU	N1-C2-N3	-9.58	120.81	128.43
56	1y	46	7MG	N3-C4-N9	9.58	139.21	126.91
56	2y	55	PSU	N1-C2-N3	-9.42	120.94	128.43
56	2y	46	7MG	N3-C4-N9	9.38	138.96	126.91
54	1w	37	MIA	C12-C13-C14	-9.06	109.52	127.14
54	2w	46	7MG	N3-C4-N9	9.01	138.48	126.91
56	2y	32	PSU	N1-C2-N3	-8.93	121.33	128.43
54	2w	55	PSU	N1-C2-N3	-8.92	121.34	128.43
56	2y	39	PSU	C4-N3-C2	8.82	122.59	115.14
55	1x	55	PSU	N1-C2-N3	-8.79	121.44	128.43
55	2x	55	PSU	N1-C2-N3	-8.75	121.47	128.43
54	1w	46	7MG	N3-C4-N9	8.75	138.15	126.91
54	1w	32	PSU	N1-C2-N3	-8.70	121.51	128.43
32	1a	527	7MG	N3-C4-N9	8.67	138.04	126.91
32	2a	516	PSU	N1-C2-N3	-8.63	121.57	128.43
1	2A	1911	PSU	N1-C2-N3	-8.48	121.69	128.43
56	1y	32	PSU	N1-C2-N3	-8.48	121.69	128.43
1	2A	1917	PSU	N1-C2-N3	-8.43	121.73	128.43
32	1a	516	PSU	N1-C2-N3	-8.39	121.76	128.43
32	2a	527	7MG	N3-C4-N9	8.33	137.61	126.91
1	1A	2605	PSU	N1-C2-N3	-8.30	121.83	128.43
56	1y	39	PSU	N1-C2-N3	-8.28	121.85	128.43
54	2w	54	5MU	C4-N3-C2	8.22	122.08	115.14
56	2y	54	5MU	C4-N3-C2	8.20	122.07	115.14
54	1w	55	PSU	N1-C2-N3	-8.19	121.92	128.43
56	2y	55	PSU	C4-N3-C2	8.17	122.04	115.14
56	1y	54	5MU	C4-N3-C2	8.16	122.03	115.14
56	1y	55	PSU	N1-C2-N3	-8.11	121.98	128.43
1	1A	1917	PSU	N1-C2-N3	-8.06	122.02	128.43
55	2x	8	4SU	C2-N3-C4	7.91	126.62	115.15
1	1A	1911	PSU	N1-C2-N3	-7.83	122.20	128.43
54	1w	39	PSU	N1-C2-N3	-7.64	122.36	128.43
55	1x	54	5MU	C4-N3-C2	7.62	121.57	115.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	1y	55	PSU	C4-N3-C2	7.59	121.55	115.14
54	2w	39	PSU	N1-C2-N3	-7.58	122.40	128.43
1	2A	2605	PSU	N1-C2-N3	-7.57	122.41	128.43
54	2w	32	PSU	C4-N3-C2	7.45	121.43	115.14
1	2A	1917	PSU	C4-N3-C2	7.33	121.33	115.14
54	1w	55	PSU	C4-N3-C2	7.20	121.22	115.14
56	2y	32	PSU	C4-N3-C2	7.16	121.19	115.14
1	2A	1915	5MU	C4-N3-C2	7.14	121.17	115.14
54	1w	32	PSU	C4-N3-C2	7.12	121.15	115.14
55	1x	55	PSU	C4-N3-C2	6.93	120.99	115.14
54	2w	55	PSU	C4-N3-C2	6.92	120.98	115.14
54	1w	54	5MU	C4-N3-C2	6.90	120.97	115.14
55	2x	55	PSU	C4-N3-C2	6.77	120.86	115.14
56	1y	39	PSU	C4-N3-C2	6.76	120.85	115.14
1	2A	1911	PSU	C4-N3-C2	6.71	120.81	115.14
1	1A	1915	5MU	C4-N3-C2	6.70	120.80	115.14
32	2a	516	PSU	C4-N3-C2	6.65	120.75	115.14
1	1A	2605	PSU	C4-N3-C2	6.63	120.74	115.14
56	1y	32	PSU	C4-N3-C2	6.53	120.66	115.14
1	1A	2503	2MA	C2-N3-C4	6.38	120.71	115.52
1	2A	2605	PSU	C4-N3-C2	6.37	120.52	115.14
56	1y	55	PSU	C5-C4-N3	-6.25	117.30	125.36
55	2x	54	5MU	C4-N3-C2	6.23	120.40	115.14
32	1a	516	PSU	C4-N3-C2	6.21	120.39	115.14
1	1A	1911	PSU	C4-N3-C2	6.16	120.34	115.14
1	2A	1939	5MU	C4-N3-C2	5.99	120.20	115.14
56	2y	46	7MG	C6-N1-C2	5.93	125.36	115.93
1	1A	1917	PSU	C4-N3-C2	5.85	120.08	115.14
32	2a	527	7MG	N7-C8-N9	-5.74	95.17	103.38
56	2y	55	PSU	C5-C4-N3	-5.73	117.98	125.36
54	1w	55	PSU	C5-C4-N3	-5.69	118.03	125.36
1	1A	2251	OMG	C2-N3-C4	5.66	121.82	115.36
55	2x	76	31H	N3-C2-N1	-5.66	119.84	128.68
1	1A	1939	5MU	C4-N3-C2	5.65	119.91	115.14
1	2A	1917	PSU	C5-C4-N3	-5.64	118.09	125.36
56	1y	46	7MG	C6-N1-C2	5.62	124.85	115.93
54	1w	76	F3N	N3-C2-N1	-5.59	119.94	128.68
54	2w	76	F3N	N3-C2-N1	-5.58	119.95	128.68
55	1x	76	31H	N3-C2-N1	-5.54	120.03	128.68
54	1w	46	7MG	N7-C8-N9	-5.52	95.49	103.38
54	1w	32	PSU	C5-C4-N3	-5.51	118.26	125.36
32	1a	527	7MG	N7-C8-N9	-5.49	95.53	103.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	2y	39	PSU	C5-C4-N3	-5.46	118.32	125.36
1	2A	2605	PSU	C5-C4-N3	-5.44	118.35	125.36
56	1y	39	PSU	C5-C4-N3	-5.43	118.36	125.36
54	1w	46	7MG	C6-N1-C2	5.42	124.55	115.93
54	2w	46	7MG	N7-C8-N9	-5.36	95.71	103.38
32	1a	966	M2G	C6-N1-C2	5.35	122.55	116.18
55	1x	55	PSU	C5-C4-N3	-5.30	118.53	125.36
56	2y	32	PSU	C5-C4-N3	-5.28	118.56	125.36
56	1y	32	PSU	C5-C4-N3	-5.27	118.57	125.36
1	2A	1911	PSU	C5-C4-N3	-5.27	118.57	125.36
56	1y	46	7MG	C5-C4-N3	-5.24	117.93	126.49
1	2A	2503	2MA	C2-N3-C4	5.22	119.76	115.52
54	2w	46	7MG	C5-C4-N3	-5.22	117.97	126.49
55	2x	55	PSU	C5-C4-N3	-5.20	118.66	125.36
1	2A	2503	2MA	C5-C6-N1	-5.17	117.63	123.06
32	1a	1207	2MG	C2-N3-C4	5.13	121.10	115.28
1	1A	2605	PSU	C5-C4-N3	-5.13	118.76	125.36
1	1A	1911	PSU	C5-C4-N3	-5.12	118.77	125.36
32	1a	516	PSU	C5-C4-N3	-5.11	118.77	125.36
54	2w	39	PSU	C4-N3-C2	5.07	119.43	115.14
56	2y	39	PSU	C5-C1'-C2'	-5.07	106.28	115.32
1	1A	2503	2MA	C5-C6-N1	-5.06	117.75	123.06
55	1x	8	4SU	C5-C4-N3	-5.06	117.07	123.83
32	1a	1519	MA6	N3-C2-N1	-5.05	120.78	128.68
54	2w	32	PSU	C5-C4-N3	-5.05	118.85	125.36
32	2a	966	M2G	C6-N1-C2	5.04	122.18	116.18
1	1A	1917	PSU	C5-C4-N3	-4.99	118.93	125.36
32	1a	527	7MG	C5-C4-N3	-4.98	118.36	126.49
56	2y	46	7MG	C5-C4-N3	-4.95	118.41	126.49
32	2a	516	PSU	C5-C4-N3	-4.94	118.99	125.36
56	2y	46	7MG	N7-C8-N9	-4.94	96.32	103.38
32	1a	966	M2G	C2-N3-C4	4.91	120.85	115.28
32	2a	966	M2G	C2-N3-C4	4.90	120.84	115.28
32	2a	1519	MA6	N3-C2-N1	-4.89	121.04	128.68
54	2w	55	PSU	C5-C1'-C2'	-4.88	106.61	115.32
1	1A	1917	PSU	C5-C6-N1	-4.87	118.45	124.44
32	1a	1518	MA6	N3-C2-N1	-4.86	121.08	128.68
54	2w	55	PSU	C5-C4-N3	-4.83	119.13	125.36
1	2A	2605	PSU	C5-C6-N1	-4.83	118.50	124.44
56	1y	46	7MG	N7-C8-N9	-4.82	96.49	103.38
54	2w	37	MIA	C11-S10-C2	-4.80	98.69	102.27
1	2A	1920	4OC	C2-N3-C4	4.73	121.14	116.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	527	7MG	C6-N1-C2	4.73	123.45	115.93
54	2w	37	MIA	C12-N6-C6	-4.71	118.81	122.87
54	1w	37	MIA	C15-C14-C13	-4.70	109.05	122.65
32	2a	1518	MA6	N3-C2-N1	-4.69	121.34	128.68
54	1w	39	PSU	C4-N3-C2	4.69	119.10	115.14
54	1w	39	PSU	C5-C4-N3	-4.67	119.34	125.36
32	2a	527	7MG	C5-C4-N3	-4.64	118.92	126.49
54	1w	39	PSU	C5-C6-N1	-4.62	118.76	124.44
54	2w	39	PSU	C5-C4-N3	-4.62	119.41	125.36
32	2a	1207	2MG	C5-C6-N1	-4.59	117.15	123.43
56	1y	8	4SU	C2-N3-C4	4.56	121.76	115.15
32	2a	1402	4OC	CM4-N4-C4	-4.55	119.06	122.97
32	1a	1207	2MG	C6-N1-C2	4.55	123.33	115.18
54	1w	46	7MG	C5-C4-N3	-4.52	119.11	126.49
54	1w	55	PSU	C5-C1'-C2'	-4.51	107.27	115.32
54	1w	39	PSU	C6-N1-C2	4.48	122.75	115.36
32	1a	516	PSU	C5-C6-N1	-4.47	118.95	124.44
54	1w	37	MIA	C2-N3-C4	4.46	121.47	115.32
32	1a	527	7MG	C6-C5-C4	4.44	119.97	115.20
1	2A	1911	PSU	C5-C6-N1	-4.44	118.98	124.44
1	1A	1917	PSU	C6-N1-C2	4.41	122.63	115.36
54	1w	8	4SU	C2-N3-C4	4.40	121.53	115.15
1	1A	2251	OMG	C6-N1-C2	4.40	122.91	115.93
32	1a	527	7MG	C6-N1-C2	4.35	122.85	115.93
32	2a	1207	2MG	C2-N3-C4	4.32	120.19	115.28
54	1w	37	MIA	C12-N6-C6	-4.32	116.15	122.55
32	1a	1207	2MG	C6-C5-C4	-4.32	116.68	120.80
32	1a	516	PSU	C6-N1-C2	4.31	122.47	115.36
54	2w	55	PSU	C6-N1-C2	4.31	122.47	115.36
1	2A	1917	PSU	C5-C1'-C2'	-4.30	107.64	115.32
56	1y	32	PSU	C5-C6-N1	-4.30	119.16	124.44
1	2A	2251	OMG	C2-N3-C4	4.29	120.26	115.36
54	2w	32	PSU	C6-N1-C2	4.29	122.44	115.36
56	1y	46	7MG	C6-C5-C4	4.28	119.80	115.20
54	2w	37	MIA	C2-N3-C4	4.28	121.22	115.32
55	1x	55	PSU	C6-N1-C2	4.28	122.42	115.36
54	2w	39	PSU	C5-C6-N1	-4.27	119.19	124.44
55	2x	55	PSU	C6-N1-C2	4.25	122.37	115.36
56	1y	32	PSU	C6-N1-C2	4.23	122.34	115.36
1	2A	2605	PSU	C5-C1'-C2'	-4.22	107.79	115.32
1	1A	1920	4OC	C2-N3-C4	4.20	120.59	116.34
54	2w	46	7MG	C6-C5-C4	4.20	119.70	115.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1207	2MG	C5-C6-N1	-4.19	117.70	123.43
1	1A	1911	PSU	C5-C6-N1	-4.18	119.31	124.44
1	2A	1917	PSU	C5-C6-N1	-4.17	119.32	124.44
55	2x	55	PSU	C5-C6-N1	-4.16	119.32	124.44
32	1a	966	M2G	C5-C6-N1	-4.16	117.74	123.43
1	2A	1911	PSU	C6-N1-C2	4.13	122.17	115.36
55	2x	8	4SU	C5-C4-N3	-4.13	118.31	123.83
56	2y	39	PSU	C6-N1-C2	4.12	122.16	115.36
54	2w	39	PSU	C6-N1-C2	4.12	122.15	115.36
32	2a	1207	2MG	C6-N1-C2	4.12	122.55	115.18
54	1w	46	7MG	C5-C6-N1	-4.11	114.69	123.14
1	2A	2605	PSU	C6-N1-C2	4.10	122.13	115.36
1	1A	1962	5MC	C2-N3-C4	4.10	120.97	116.02
1	1A	2251	OMG	N3-C2-N1	-4.09	121.76	127.22
1	1A	1911	PSU	C6-N1-C2	4.09	122.11	115.36
1	1A	2251	OMG	C5-C6-N1	-4.08	117.85	123.43
56	2y	32	PSU	C6-N1-C2	4.07	122.07	115.36
32	2a	1404	5MC	C2-N3-C4	4.07	120.93	116.02
32	2a	516	PSU	C6-N1-C2	4.05	122.05	115.36
54	2w	46	7MG	C6-N1-C2	4.05	122.36	115.93
54	1w	46	7MG	C6-C5-C4	4.05	119.55	115.20
56	2y	46	7MG	C5-C6-N1	-4.03	114.86	123.14
32	2a	966	M2G	C5-C6-N1	-4.02	117.93	123.43
56	1y	39	PSU	C6-N1-C2	4.02	121.99	115.36
32	1a	966	M2G	C6-C5-C4	-4.00	116.98	120.80
56	2y	8	4SU	C2-N3-C4	4.00	120.94	115.15
54	2w	55	PSU	C5-C6-N1	-3.99	119.53	124.44
1	2A	1917	PSU	C6-N1-C2	3.99	121.94	115.36
32	1a	1400	5MC	C2-N3-C4	3.97	120.81	116.02
55	1x	55	PSU	C5-C6-N1	-3.97	119.56	124.44
56	1y	46	7MG	C5-C6-N1	-3.95	115.02	123.14
56	2y	46	7MG	C6-C5-C4	3.95	119.44	115.20
1	1A	2605	PSU	C5-C1'-C2'	-3.91	108.34	115.32
1	2A	2251	OMG	C6-C5-C4	-3.90	117.07	120.80
32	1a	527	7MG	C5-C6-N1	-3.89	115.16	123.14
1	1A	2605	PSU	C6-N1-C2	3.87	121.75	115.36
1	1A	2605	PSU	C5-C6-N1	-3.87	119.69	124.44
56	1y	39	PSU	C5-C6-N1	-3.87	119.69	124.44
32	2a	516	PSU	C5-C6-N1	-3.85	119.70	124.44
54	1w	32	PSU	C6-N1-C2	3.85	121.72	115.36
32	2a	527	7MG	C5-C6-N1	-3.84	115.26	123.14
32	2a	1207	2MG	CM2-N2-C2	-3.82	118.98	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1207	2MG	C6-C5-C4	-3.80	117.17	120.80
1	2A	2251	OMG	C6-N1-C2	3.79	121.95	115.93
54	1w	37	MIA	C16-C14-C13	-3.75	111.82	122.65
32	1a	1407	5MC	C2-N3-C4	3.74	120.54	116.02
56	2y	37	MIA	N3-C2-N1	-3.70	122.89	128.68
32	1a	1402	4OC	CM4-N4-C4	-3.70	119.79	122.97
32	1a	1404	5MC	C2-N3-C4	3.68	120.47	116.02
54	2w	32	PSU	C5-C6-N1	-3.65	119.95	124.44
55	1x	32	5MC	C2-N3-C4	3.65	120.42	116.02
56	2y	39	PSU	C5-C6-N1	-3.65	119.96	124.44
1	2A	2251	OMG	C5-C6-N1	-3.63	118.47	123.43
54	1w	55	PSU	C6-N1-C2	3.62	121.34	115.36
54	1w	32	PSU	C5-C6-N1	-3.62	119.99	124.44
32	2a	527	7MG	C6-C5-C4	3.60	119.06	115.20
1	1A	1939	5MU	C5-C6-N1	-3.60	118.32	122.19
54	2w	8	4SU	C2-N3-C4	3.57	120.33	115.15
56	2y	55	PSU	C6-N1-C2	3.54	121.19	115.36
1	2A	1962	5MC	C2-N3-C4	3.54	120.29	116.02
54	2w	46	7MG	C5-C6-N1	-3.51	115.93	123.14
55	2x	32	5MC	C2-N3-C4	3.50	120.24	116.02
54	2w	37	MIA	C5-C6-N1	-3.50	117.91	120.81
32	2a	967	5MC	C2-N3-C4	3.49	120.24	116.02
56	2y	32	PSU	C5-C6-N1	-3.48	120.17	124.44
32	2a	1400	5MC	C2-N3-C4	3.47	120.20	116.02
56	1y	55	PSU	C6-N1-C2	3.43	121.02	115.36
32	1a	1207	2MG	C4-C5-N7	-3.43	105.82	109.40
1	1A	1917	PSU	C5-C1'-C2'	-3.43	109.20	115.32
32	2a	1519	MA6	C4-C5-N7	-3.37	105.88	109.40
32	2a	1407	5MC	C2-N3-C4	3.35	120.07	116.02
1	1A	1942	5MC	N4-C4-N3	3.35	121.77	117.03
1	2A	1911	PSU	C5-C1'-C2'	-3.35	109.34	115.32
32	2a	1207	2MG	C4-C5-N7	-3.35	105.91	109.40
55	1x	32	5MC	N4-C4-N3	3.35	121.76	117.03
1	1A	2251	OMG	C6-C5-C4	-3.33	117.61	120.80
32	1a	967	5MC	C2-N3-C4	3.31	120.01	116.02
1	1A	1942	5MC	C2-N3-C4	3.29	119.99	116.02
56	1y	37	MIA	N3-C2-N1	-3.25	123.59	128.68
56	1y	55	PSU	C5-C6-N1	-3.21	120.50	124.44
54	1w	55	PSU	C5-C6-N1	-3.20	120.51	124.44
56	1y	32	PSU	C5-C1'-C2'	-3.19	109.63	115.32
1	2A	1939	5MU	C5-C6-N1	-3.18	118.77	122.19
32	2a	966	M2G	C6-C5-C4	-3.17	117.77	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	966	M2G	C4-C5-N7	-3.15	106.12	109.40
1	2A	1942	5MC	C2-N3-C4	3.13	119.80	116.02
56	1y	8	4SU	C5-C4-N3	-3.07	119.72	123.83
1	1A	2251	OMG	C4-C5-N7	-3.04	106.23	109.40
32	1a	1400	5MC	N4-C4-N3	3.03	121.32	117.03
32	1a	1518	MA6	C4-C5-N7	-3.03	106.24	109.40
32	2a	1518	MA6	C4-C5-N7	-3.01	106.27	109.40
54	2w	8	4SU	C5-C4-N3	-2.99	119.82	123.83
32	1a	1519	MA6	C4-C5-N7	-2.99	106.28	109.40
1	2A	1962	5MC	N4-C4-N3	2.96	121.21	117.03
1	2A	2251	OMG	N3-C2-N1	-2.93	123.31	127.22
32	2a	527	7MG	C8-N7-C5	2.92	116.54	108.94
54	1w	37	MIA	C4-C5-N7	-2.92	106.36	109.40
54	1w	37	MIA	C5-C6-N1	-2.88	118.42	120.81
32	1a	1404	5MC	N4-C4-N3	2.87	121.10	117.03
56	2y	8	4SU	C5-C4-N3	-2.87	119.99	123.83
54	1w	8	4SU	C5-C4-N3	-2.86	120.01	123.83
1	2A	2503	2MA	C4-C5-N7	-2.82	106.46	109.40
54	2w	55	PSU	O4'-C1'-C5	2.79	114.25	109.93
55	2x	32	5MC	N4-C4-N3	2.78	120.96	117.03
32	2a	1404	5MC	N4-C4-N3	2.78	120.96	117.03
32	1a	527	7MG	C8-N7-C5	2.76	116.11	108.94
54	2w	46	7MG	C8-N7-C5	2.75	116.08	108.94
56	2y	46	7MG	C5-C4-N9	-2.74	102.61	106.44
55	2x	32	5MC	C5-C6-N1	-2.74	119.25	122.19
54	2w	39	PSU	C5-C1'-C2'	-2.73	110.46	115.32
54	1w	37	MIA	C2-N1-C6	2.71	122.04	117.19
56	2y	37	MIA	C4-C5-N7	-2.70	106.59	109.40
1	2A	1942	5MC	C5-C6-N1	-2.67	119.31	122.19
55	1x	32	5MC	CM5-C5-C4	-2.66	119.03	121.72
54	1w	46	7MG	C8-N7-C5	2.65	115.84	108.94
54	1w	46	7MG	C5-C4-N9	-2.64	102.74	106.44
32	2a	1400	5MC	C5-C6-N1	-2.64	119.35	122.19
56	1y	37	MIA	C4-C5-N7	-2.61	106.67	109.40
56	1y	39	PSU	C5-C1'-C2'	-2.59	110.70	115.32
32	2a	967	5MC	C5-C6-N1	-2.59	119.41	122.19
54	1w	37	MIA	N3-C2-N1	-2.56	122.27	126.98
55	2x	55	PSU	C5-C1'-C2'	-2.56	110.75	115.32
56	1y	46	7MG	C5-C4-N9	-2.56	102.86	106.44
54	2w	37	MIA	C4-C5-N7	-2.55	106.74	109.40
32	1a	1207	2MG	N3-C2-N1	-2.54	122.22	126.23
32	1a	1207	2MG	CM2-N2-C2	-2.53	120.53	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1942	5MC	C5-C6-N1	-2.52	119.48	122.19
56	2y	46	7MG	C8-N7-C5	2.51	115.47	108.94
55	1x	32	5MC	C5-C6-N1	-2.50	119.50	122.19
56	1y	46	7MG	C8-N7-C5	2.48	115.40	108.94
54	2w	37	MIA	C2-N1-C6	2.48	121.62	117.19
32	1a	1498	UR3	C3U-N3-C4	2.45	121.37	118.12
55	1x	76	31H	O4'-C1'-C2'	-2.44	103.36	106.93
55	2x	76	31H	O4'-C1'-C2'	-2.43	103.37	106.93
55	1x	55	PSU	C5-C1'-C2'	-2.41	111.01	115.32
32	1a	1407	5MC	N4-C4-N3	2.39	120.42	117.03
55	2x	54	5MU	C5-C6-N1	-2.38	119.63	122.19
32	2a	1498	UR3	C3U-N3-C4	2.37	121.26	118.12
32	1a	967	5MC	N4-C4-N3	2.36	120.37	117.03
32	2a	967	5MC	N4-C4-N3	2.36	120.37	117.03
32	2a	1407	5MC	C5-C6-N1	-2.36	119.65	122.19
32	2a	1407	5MC	N4-C4-N3	2.36	120.36	117.03
55	2x	32	5MC	CM5-C5-C4	-2.35	119.34	121.72
55	1x	76	31H	O2'-C2'-C3'	2.34	116.90	111.16
1	2A	1942	5MC	N4-C4-N3	2.31	120.30	117.03
54	1w	32	PSU	C5-C1'-C2'	-2.31	111.20	115.32
32	1a	966	M2G	CM2-N2-C2	-2.31	119.09	121.29
1	1A	1915	5MU	C5-C6-N1	-2.28	119.73	122.19
56	1y	46	7MG	C2-N3-C4	2.26	120.13	113.89
32	1a	1207	2MG	N2-C2-N3	2.25	119.12	116.96
54	2w	76	F3N	C3'-N3'-C	-2.24	119.83	123.21
32	2a	1207	2MG	N2-C2-N1	2.23	119.10	116.96
1	1A	1920	4OC	N4-C4-N3	2.23	120.01	116.49
54	2w	37	MIA	C1'-N9-C4	2.23	130.55	126.64
54	2w	46	7MG	C2-N3-C4	2.21	120.01	113.89
54	1w	54	5MU	C5-C6-N1	-2.20	119.83	122.19
56	2y	46	7MG	O4'-C1'-N9	-2.18	106.40	109.35
54	2w	32	PSU	O4'-C1'-C5	2.18	113.30	109.93
32	1a	516	PSU	O4'-C1'-C2'	2.16	108.16	104.66
1	1A	2552	2MU	C5-C4-N3	-2.16	118.56	123.31
56	2y	55	PSU	C5-C1'-C2'	-2.16	111.47	115.32
1	2A	1962	5MC	C5-C6-N1	-2.16	119.87	122.19
56	2y	55	PSU	C5-C6-N1	-2.15	121.80	124.44
56	2y	46	7MG	C2-N3-C4	2.14	119.81	113.89
32	2a	527	7MG	C5-C4-N9	-2.12	103.47	106.44
32	2a	966	M2G	N3-C2-N2	2.12	119.33	117.18
56	2y	46	7MG	N1-C2-N3	-2.11	122.11	125.42
32	2a	1400	5MC	N4-C4-N3	2.11	120.01	117.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	516	PSU	C5-C1'-C2'	-2.10	111.56	115.32
54	1w	39	PSU	C5-C1'-C2'	-2.10	111.57	115.32
55	1x	76	31H	OCN-CN-N	-2.09	119.75	125.27
32	2a	527	7MG	C2-N3-C4	2.09	119.68	113.89
54	2w	46	7MG	C5-C4-N9	-2.07	103.55	106.44
55	2x	76	31H	O2'-C2'-C3'	2.06	116.22	111.16
1	2A	2552	2MU	C5-C4-N3	-2.05	118.79	123.31
32	1a	1519	MA6	C1'-N9-C4	-2.05	123.04	126.64
56	1y	55	PSU	O4'-C1'-C2'	2.04	107.97	104.66
32	1a	527	7MG	C5-C4-N9	-2.04	103.59	106.44
32	1a	1404	5MC	C5-C6-N1	-2.04	120.00	122.19
55	1x	76	31H	CA-N-CN	-2.03	119.70	122.82
32	2a	527	7MG	CM7-N7-C5	2.03	131.80	124.01
56	2y	37	MIA	C2-N1-C6	2.03	122.22	118.75
56	1y	46	7MG	N1-C2-N3	-2.01	122.26	125.42
32	2a	516	PSU	O4'-C1'-C2'	2.01	107.91	104.66
54	1w	37	MIA	C11-S10-C2	-2.00	100.77	102.27
56	2y	46	7MG	CM7-N7-C5	2.00	131.71	124.01

There are no chirality outliers.

All (73) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1A	1962	5MC	O4'-C1'-N1-C6
1	1A	1962	5MC	C2'-C1'-N1-C6
55	1x	76	31H	C3'-C4'-C5'-O5'
32	1a	1207	2MG	N1-C2-N2-CM2
32	1a	1207	2MG	N3-C2-N2-CM2
32	2a	1402	4OC	C5-C4-N4-CM4
1	2A	2251	OMG	C1'-C2'-O2'-CM2
32	1a	1519	MA6	O4'-C4'-C5'-O5'
43	1l	92	0TD	CG-CB-SB-CSB
56	2y	54	5MU	C3'-C4'-C5'-O5'
56	1y	8	4SU	O4'-C1'-N1-C6
1	2A	1962	5MC	O4'-C1'-N1-C6
1	2A	1962	5MC	C2'-C1'-N1-C6
56	2y	37	MIA	C3'-C4'-C5'-O5'
55	2x	76	31H	C3'-C4'-C5'-O5'
56	2y	55	PSU	C3'-C4'-C5'-O5'
54	1w	37	MIA	C12-C13-C14-C15
54	1w	37	MIA	C12-C13-C14-C16
56	1y	46	7MG	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
1	1A	1920	4OC	O4'-C1'-N1-C6
55	2x	76	31H	CB-CG-SD-CE
32	1a	1519	MA6	C3'-C4'-C5'-O5'
56	2y	54	5MU	O4'-C4'-C5'-O5'
32	2a	1519	MA6	O4'-C4'-C5'-O5'
56	1y	37	MIA	C3'-C4'-C5'-O5'
55	1x	76	31H	O4'-C4'-C5'-O5'
32	2a	527	7MG	C3'-C4'-C5'-O5'
55	2x	76	31H	O4'-C4'-C5'-O5'
1	2A	1917	PSU	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
56	2y	37	MIA	O4'-C4'-C5'-O5'
32	2a	527	7MG	O4'-C4'-C5'-O5'
56	1y	37	MIA	O4'-C4'-C5'-O5'
56	2y	55	PSU	O4'-C4'-C5'-O5'
32	2a	1402	4OC	O4'-C4'-C5'-O5'
32	2a	1498	UR3	O4'-C4'-C5'-O5'
56	1y	8	4SU	O4'-C4'-C5'-O5'
56	2y	46	7MG	O4'-C1'-N9-C4
55	1x	76	31H	C4'-C5'-O5'-P
56	1y	46	7MG	C2'-C1'-N9-C8
56	2y	46	7MG	C2'-C1'-N9-C8
32	2a	527	7MG	C4'-C5'-O5'-P
32	2a	1498	UR3	C3'-C4'-C5'-O5'
56	1y	8	4SU	C3'-C4'-C5'-O5'
54	1w	46	7MG	C2'-C1'-N9-C8
32	1a	527	7MG	C3'-C4'-C5'-O5'
1	2A	1917	PSU	C3'-C4'-C5'-O5'
56	2y	46	7MG	O4'-C1'-N9-C8
32	1a	527	7MG	C4'-C5'-O5'-P
32	2a	1519	MA6	C4'-C5'-O5'-P
54	1w	46	7MG	C4'-C5'-O5'-P
54	2w	37	MIA	N3-C2-S10-C11
56	1y	46	7MG	C3'-C4'-C5'-O5'
54	1w	37	MIA	N6-C12-C13-C14
1	2A	2503	2MA	O4'-C4'-C5'-O5'
56	2y	55	PSU	O4'-C1'-C5-C6
54	2w	37	MIA	N1-C2-S10-C11
32	1a	1402	4OC	C3'-C2'-O2'-CM2
56	2y	55	PSU	O4'-C1'-C5-C4
43	2l	92	0TD	CA-CB-SB-CSB
32	1a	967	5MC	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
32	1a	1400	5MC	O4'-C4'-C5'-O5'
56	1y	46	7MG	O4'-C1'-N9-C8
54	2w	32	PSU	C2'-C1'-C5-C6
1	1A	2503	2MA	C4'-C5'-O5'-P
32	2a	1402	4OC	C3'-C4'-C5'-O5'
32	1a	1402	4OC	O4'-C4'-C5'-O5'
56	1y	46	7MG	C2'-C1'-N9-C4
54	1w	46	7MG	O4'-C1'-N9-C8
43	2l	92	0TD	CG-CB-SB-CSB
32	1a	1400	5MC	C3'-C4'-C5'-O5'
1	1A	2503	2MA	O4'-C4'-C5'-O5'
56	2y	37	MIA	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 2812 ligands modelled in this entry, 2810 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	0.00	-	-		
60	SF4	2d	501	35	0,12,12	0.00	-	-		

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	501	35	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.60	126 (4%)	34	37	15, 31, 83, 96	0
1	2A	2789/2915 (95%)	0.41	108 (3%)	39	42	27, 50, 81, 93	0
2	1B	120/121 (99%)	0.22	0	100	100	24, 41, 55, 75	0
2	2B	120/121 (99%)	0.08	0	100	100	56, 66, 73, 77	0
3	1D	275/276 (99%)	0.59	2 (0%)	87	89	17, 33, 46, 63	0
3	2D	275/276 (99%)	0.67	8 (2%)	51	55	26, 45, 56, 77	0
4	1E	204/206 (99%)	0.57	2 (0%)	82	84	16, 37, 54, 61	0
4	2E	204/206 (99%)	0.54	2 (0%)	82	84	25, 52, 63, 72	0
5	1F	203/210 (96%)	0.55	0	100	100	16, 37, 58, 70	0
5	2F	203/210 (96%)	0.58	4 (1%)	65	68	28, 59, 70, 80	0
6	1G	181/182 (99%)	0.43	5 (2%)	53	56	31, 50, 63, 73	0
6	2G	181/182 (99%)	0.73	14 (7%)	13	13	56, 67, 74, 79	0
7	1H	174/180 (96%)	0.44	1 (0%)	89	90	33, 48, 58, 64	0
7	2H	174/180 (96%)	1.13	30 (17%)	1	1	58, 70, 77, 83	0
8	1I	146/148 (98%)	0.29	1 (0%)	87	89	35, 63, 72, 76	0
8	2I	146/148 (98%)	0.79	16 (10%)	5	5	49, 67, 77, 83	0
9	1N	140/140 (100%)	0.60	1 (0%)	87	89	23, 34, 53, 66	0
9	2N	140/140 (100%)	0.63	8 (5%)	23	25	35, 56, 68, 79	0
10	1O	122/122 (100%)	0.50	0	100	100	24, 37, 51, 58	0
10	2O	122/122 (100%)	0.48	1 (0%)	86	87	36, 49, 61, 66	0
11	1P	149/150 (99%)	0.53	2 (1%)	77	79	15, 40, 62, 69	0
11	2P	149/150 (99%)	0.79	13 (8%)	10	10	34, 58, 72, 81	0
12	1Q	141/141 (100%)	0.59	1 (0%)	87	89	18, 34, 47, 58	0
12	2Q	141/141 (100%)	0.91	12 (8%)	10	10	33, 55, 65, 68	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	0.59	0 100 100	22, 30, 41, 50	0
13	2R	118/118 (100%)	0.56	2 (1%) 70 72	35, 45, 58, 61	0
14	1S	110/112 (98%)	0.39	0 100 100	30, 41, 52, 57	0
14	2S	110/112 (98%)	0.48	4 (3%) 42 46	51, 61, 68, 72	0
15	1T	131/146 (89%)	0.53	2 (1%) 73 75	29, 39, 61, 72	0
15	2T	131/146 (89%)	0.49	2 (1%) 73 75	42, 53, 66, 72	0
16	1U	116/118 (98%)	0.62	1 (0%) 84 86	18, 26, 42, 55	0
16	2U	116/118 (98%)	0.64	4 (3%) 45 48	38, 52, 63, 69	0
17	1V	101/101 (100%)	0.51	0 100 100	16, 35, 48, 56	0
17	2V	101/101 (100%)	0.55	4 (3%) 38 41	37, 61, 68, 74	0
18	1W	112/113 (99%)	0.61	1 (0%) 84 86	20, 29, 46, 75	0
18	2W	112/113 (99%)	0.77	3 (2%) 54 58	36, 45, 59, 74	0
19	1X	95/96 (98%)	0.47	0 100 100	21, 32, 51, 70	0
19	2X	95/96 (98%)	0.77	7 (7%) 14 15	39, 53, 66, 70	0
20	1Y	107/110 (97%)	0.44	0 100 100	30, 44, 58, 68	0
20	2Y	107/110 (97%)	1.09	21 (19%) 1 1	51, 62, 72, 79	0
21	1Z	154/206 (74%)	0.55	6 (3%) 39 42	29, 53, 69, 72	0
21	2Z	160/206 (77%)	1.09	27 (16%) 1 1	55, 68, 76, 83	0
22	10	83/85 (97%)	0.63	0 100 100	22, 29, 43, 54	0
22	20	83/85 (97%)	0.88	4 (4%) 30 32	36, 53, 61, 67	0
23	11	97/98 (98%)	0.54	3 (3%) 49 52	22, 40, 60, 66	0
23	21	97/98 (98%)	0.81	6 (6%) 20 21	36, 52, 66, 70	0
24	12	70/72 (97%)	0.54	0 100 100	28, 43, 51, 58	0
24	22	70/72 (97%)	0.49	0 100 100	53, 60, 67, 72	0
25	13	59/60 (98%)	0.49	0 100 100	17, 31, 53, 67	0
25	23	59/60 (98%)	0.72	3 (5%) 28 29	48, 56, 71, 78	0
26	14	69/71 (97%)	0.55	7 (10%) 7 6	43, 64, 77, 82	0
26	24	69/71 (97%)	1.30	17 (24%) 0 0	66, 73, 81, 85	0
27	15	59/60 (98%)	0.61	1 (1%) 70 72	17, 28, 43, 54	0
27	25	59/60 (98%)	0.61	2 (3%) 45 48	32, 45, 57, 72	0
28	16	53/54 (98%)	0.53	0 100 100	27, 35, 48, 51	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.74	2 (3%) 40 43	42, 52, 58, 61	0
29	17	48/49 (97%)	0.89	6 (12%) 3 3	17, 24, 45, 53	0
29	27	48/49 (97%)	1.05	4 (8%) 11 11	29, 37, 54, 66	0
30	18	64/65 (98%)	0.55	0 100 100	22, 29, 37, 43	0
30	28	64/65 (98%)	0.88	3 (4%) 31 33	38, 49, 54, 58	0
31	19	37/37 (100%)	0.65	0 100 100	27, 35, 44, 48	0
31	29	37/37 (100%)	0.89	2 (5%) 25 27	48, 57, 64, 65	0
32	1a	1488/1521 (97%)	0.26	31 (2%) 63 66	28, 55, 80, 91	0
32	2a	1491/1521 (98%)	0.43	58 (3%) 39 42	44, 66, 82, 95	0
33	1b	231/256 (90%)	0.64	13 (5%) 24 25	53, 64, 74, 80	0
33	2b	231/256 (90%)	1.41	52 (22%) 0 0	63, 72, 77, 82	0
34	1c	206/239 (86%)	0.79	16 (7%) 13 13	45, 58, 69, 75	0
34	2c	206/239 (86%)	1.26	41 (19%) 1 1	61, 71, 76, 82	0
35	1d	208/209 (99%)	0.56	7 (3%) 45 48	43, 57, 66, 71	0
35	2d	208/209 (99%)	1.06	32 (15%) 2 1	55, 64, 72, 76	0
36	1e	148/162 (91%)	0.72	9 (6%) 21 22	41, 54, 65, 75	0
36	2e	148/162 (91%)	1.06	23 (15%) 2 1	58, 66, 71, 75	0
37	1f	100/101 (99%)	0.42	1 (1%) 82 84	43, 52, 65, 69	0
37	2f	100/101 (99%)	0.46	2 (2%) 65 68	51, 59, 67, 70	0
38	1g	155/156 (99%)	0.65	13 (8%) 11 11	49, 61, 73, 84	0
38	2g	155/156 (99%)	1.23	33 (21%) 0 0	61, 69, 75, 79	0
39	1h	137/138 (99%)	0.72	6 (4%) 34 37	46, 56, 63, 70	0
39	2h	137/138 (99%)	1.35	31 (22%) 0 0	57, 67, 72, 77	0
40	1i	127/128 (99%)	0.72	8 (6%) 20 21	43, 62, 71, 78	0
40	2i	127/128 (99%)	2.09	57 (44%) 0 0	62, 71, 77, 79	0
41	1j	97/105 (92%)	0.90	8 (8%) 11 11	45, 64, 72, 79	0
41	2j	96/105 (91%)	1.70	37 (38%) 0 0	65, 72, 77, 78	0
42	1k	114/129 (88%)	0.68	7 (6%) 21 22	34, 58, 67, 71	0
42	2k	114/129 (88%)	0.67	8 (7%) 16 16	50, 63, 70, 72	0
43	1l	121/132 (91%)	0.55	2 (1%) 70 72	37, 45, 57, 65	0
43	2l	121/132 (91%)	0.81	11 (9%) 9 9	46, 56, 63, 66	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	123/126 (97%)	0.68	9 (7%) 15 15	43, 57, 65, 77	0
44	2m	122/126 (96%)	1.29	30 (24%) 0 0	60, 70, 74, 76	0
45	1n	60/61 (98%)	0.93	5 (8%) 11 11	42, 53, 60, 63	0
45	2n	60/61 (98%)	2.38	34 (56%) 0 0	60, 70, 75, 76	0
46	1o	88/89 (98%)	0.53	1 (1%) 80 82	35, 54, 64, 66	0
46	2o	88/89 (98%)	0.99	14 (15%) 1 1	46, 63, 70, 74	0
47	1p	82/88 (93%)	1.18	12 (14%) 2 2	47, 60, 66, 71	0
47	2p	82/88 (93%)	0.81	5 (6%) 21 22	52, 60, 67, 74	0
48	1q	99/105 (94%)	0.80	6 (6%) 21 22	45, 58, 65, 68	0
48	2q	99/105 (94%)	1.45	28 (28%) 0 0	56, 63, 70, 74	0
49	1r	68/88 (77%)	0.52	2 (2%) 51 55	45, 55, 64, 66	0
49	2r	68/88 (77%)	0.71	3 (4%) 34 37	56, 64, 72, 76	0
50	1s	83/93 (89%)	0.57	4 (4%) 30 32	48, 58, 67, 72	0
50	2s	83/93 (89%)	1.43	26 (31%) 0 0	63, 71, 75, 81	0
51	1t	96/106 (90%)	0.92	17 (17%) 1 1	52, 60, 67, 75	0
51	2t	96/106 (90%)	0.91	10 (10%) 6 6	48, 61, 70, 76	0
52	1u	23/27 (85%)	1.13	4 (17%) 1 1	49, 56, 63, 66	0
52	2u	23/27 (85%)	2.17	10 (43%) 0 0	64, 70, 72, 79	0
53	1v	13/24 (54%)	1.16	3 (23%) 0 0	36, 41, 79, 87	0
53	2v	13/24 (54%)	1.75	6 (46%) 0 0	55, 63, 85, 91	0
54	1w	66/76 (86%)	0.76	7 (10%) 6 5	23, 71, 84, 89	0
54	2w	64/76 (84%)	0.97	11 (17%) 1 1	37, 78, 85, 90	0
55	1x	71/77 (92%)	0.26	0 100 100	19, 50, 69, 82	0
55	2x	71/77 (92%)	0.27	1 (1%) 75 77	32, 65, 75, 84	0
56	1y	67/76 (88%)	3.54	56 (83%) 0 0	55, 85, 89, 92	0
56	2y	66/76 (86%)	4.06	60 (90%) 0 0	64, 86, 90, 91	0
All	All	20871/21748 (95%)	0.65	1371 (6%) 18 19	15, 54, 77, 96	0

All (1371) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
44	1m	124	PRO	11.6
44	2m	124	PRO	10.8

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Mol	Chain	Res	Type	RSRZ
56	1y	35	A	9.2
44	2m	123	ALA	9.2
21	2Z	149	SER	9.0
56	1y	36	A	9.0
54	2w	71	G	8.8
54	1w	70	G	8.7
56	2y	36	A	8.7
38	2g	81	GLY	8.3
56	2y	29	G	8.2
32	2a	1030(B)	C	8.0
38	1g	81	GLY	7.9
56	1y	1	G	7.7
54	2w	70	G	7.7
1	2A	885	C	7.6
40	2i	109	VAL	7.5
1	1A	2145	C	7.5
1	2A	883	G	7.4
56	1y	34	G	7.4
1	2A	2146	C	7.3
56	2y	65	G	7.3
45	2n	42	ILE	7.3
21	2Z	141	VAL	7.3
1	1A	2140	C	7.3
1	1A	2159	G	6.9
34	2c	87	LEU	6.9
56	2y	74	C	6.8
56	2y	14	A	6.8
1	1A	2112	G	6.8
56	2y	34	G	6.8
32	2a	1030(A)	G	6.8
1	1A	2161	C	6.7
1	2A	884	C	6.5
1	1A	2109	U	6.4
1	2A	2127	G	6.4
33	2b	81	VAL	6.4
21	2Z	148	ASP	6.4
48	2q	80	GLY	6.3
1	1A	2131	G	6.3
38	2g	154	TYR	6.2
44	2m	122	LYS	6.2
38	1g	156	TRP	6.2
38	2g	80	VAL	6.1

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Mol	Chain	Res	Type	RSRZ
56	1y	5	G	6.1
56	2y	1	G	6.1
1	2A	2141	G	6.1
32	2a	1034	G	6.0
54	1w	71	G	6.0
1	1A	2130	U	6.0
56	2y	22	G	6.0
50	2s	49	ILE	6.0
21	2Z	155	LEU	6.0
54	2w	72	C	5.9
56	2y	35	A	5.9
1	2A	2110	G	5.9
33	2b	165	VAL	5.8
56	2y	38	A	5.8
3	2D	2	ALA	5.8
40	2i	76	ALA	5.8
23	21	2	SER	5.7
26	24	66	SER	5.7
56	1y	75	C	5.7
56	2y	15	G	5.7
50	2s	79	THR	5.7
45	2n	34	TYR	5.7
1	1A	1096	A	5.7
20	2Y	55	TYR	5.6
26	24	50	VAL	5.6
38	2g	40	ALA	5.6
56	1y	13	C	5.6
36	2e	123	LEU	5.6
1	1A	2111	C	5.6
1	1A	2181	G	5.6
44	2m	119	GLY	5.6
44	1m	123	ALA	5.6
1	2A	2128	C	5.6
56	2y	21	A	5.6
1	1A	1509	C	5.6
45	2n	10	ALA	5.5
1	1A	2141	G	5.5
1	1A	885	C	5.5
1	2A	2145	C	5.5
32	2a	1036	G	5.5
1	2A	2147	G	5.5
45	2n	39	LEU	5.5

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Mol	Chain	Res	Type	RSRZ
1	1A	2129	C	5.4
40	2i	14	VAL	5.4
56	1y	62	C	5.4
7	2H	35	VAL	5.4
38	1g	80	VAL	5.4
1	1A	884	C	5.4
1	1A	2160	G	5.4
1	1A	2115	G	5.3
38	2g	32	ARG	5.3
7	2H	72	ILE	5.3
51	1t	95	ALA	5.3
1	2A	2142	C	5.3
9	2N	8	GLN	5.3
38	2g	156	TRP	5.3
56	1y	71	G	5.3
38	2g	79	ARG	5.3
56	2y	62	C	5.2
56	2y	44	G	5.2
33	2b	215	LEU	5.2
41	2j	66	ARG	5.2
53	2v	12	A	5.2
32	2a	1033	G	5.2
40	2i	30	GLY	5.2
56	2y	75	C	5.2
52	2u	17	THR	5.2
1	1A	888	C	5.2
1	2A	2802	G	5.2
56	1y	19	G	5.2
33	2b	127	ILE	5.2
32	2a	1531	A	5.1
33	2b	207	ALA	5.1
40	2i	52	ALA	5.1
56	2y	28	G	5.1
38	2g	82	GLY	5.1
56	2y	64	A	5.0
1	2A	2112	G	5.0
40	2i	17	VAL	5.0
1	2A	2160	G	5.0
1	1A	2146	C	5.0
1	2A	2174	C	5.0
20	2Y	1	MET	5.0
1	2A	2115	G	4.9

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Mol	Chain	Res	Type	RSRZ
50	2s	80	TYR	4.9
32	2a	1030	C	4.9
1	2A	896	A	4.9
40	2i	90	PRO	4.9
45	2n	38	GLY	4.9
32	2a	1027	C	4.9
34	2c	8	ILE	4.9
34	1c	65	ALA	4.9
26	24	63	TYR	4.9
32	2a	1031	G	4.9
39	2h	58	TYR	4.9
21	2Z	144	LEU	4.9
7	2H	99	VAL	4.9
56	2y	52	G	4.8
56	2y	66	U	4.8
50	2s	50	ALA	4.8
1	2A	1509	C	4.8
1	1A	2147	G	4.8
1	2A	2155	G	4.8
1	1A	887	A	4.8
34	1c	100	ALA	4.8
33	2b	232	PRO	4.8
1	2A	2138	C	4.8
33	2b	121	LEU	4.8
56	2y	23	A	4.8
47	1p	1	MET	4.8
41	2j	38	ILE	4.8
47	1p	19	ILE	4.8
8	2I	83	ALA	4.7
56	2y	10	G	4.7
33	2b	113	HIS	4.7
1	2A	2154	G	4.7
8	2I	75	LEU	4.7
21	2Z	152	ALA	4.7
1	1A	2120	G	4.7
52	2u	11	GLY	4.7
19	2X	92	LEU	4.7
40	2i	8	GLY	4.6
33	2b	34	ALA	4.6
32	1a	1531	A	4.6
26	24	52	THR	4.6
56	2y	33	U	4.6

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Mol	Chain	Res	Type	RSRZ
42	2k	25	TYR	4.6
56	1y	70	G	4.6
56	1y	38	A	4.6
21	2Z	96	VAL	4.6
45	2n	35	ARG	4.6
1	1A	889	C	4.6
36	2e	90	VAL	4.6
40	2i	36	TYR	4.6
1	1A	2132	U	4.5
1	1A	2144	U	4.5
56	1y	24	G	4.5
1	1A	2143	C	4.5
1	2A	2143	C	4.5
1	1A	2110	G	4.5
40	2i	115	GLY	4.5
32	2a	1532	U	4.5
36	2e	12	LEU	4.5
56	2y	13	C	4.5
29	27	1	MET	4.5
32	2a	1035	A	4.5
1	1A	2162	G	4.4
1	2A	2111	C	4.4
56	2y	42	C	4.4
41	1j	38	ILE	4.4
26	24	51	ASP	4.4
28	26	52	VAL	4.4
40	2i	72	GLY	4.4
1	2A	888	C	4.4
1	2A	2133	G	4.4
41	1j	20	ALA	4.4
56	2y	70	G	4.4
14	2S	32	LEU	4.4
52	2u	13	ILE	4.4
1	2A	2803	C	4.4
41	2j	72	VAL	4.4
56	2y	5	G	4.4
56	2y	57	G	4.3
44	2m	120	LYS	4.3
1	1A	2119	A	4.3
56	1y	23	A	4.3
7	2H	115	VAL	4.3
21	2Z	170	THR	4.3

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Mol	Chain	Res	Type	RSRZ
40	2i	125	TYR	4.3
1	2A	2179	C	4.3
56	1y	2	C	4.3
34	2c	39	ILE	4.3
1	1A	2128	C	4.3
51	1t	13	LEU	4.3
1	2A	2793	G	4.3
1	2A	2804	C	4.3
19	2X	69	TYR	4.3
40	2i	113	LYS	4.3
1	1A	897	C	4.2
32	1a	1036	G	4.2
41	2j	65	LEU	4.2
38	2g	147	ALA	4.2
1	2A	886	C	4.2
1	2A	2123	G	4.2
44	2m	78	ILE	4.2
1	2A	2109	U	4.2
33	2b	187	LEU	4.2
32	2a	1001(A)	G	4.2
34	2c	60	ALA	4.2
26	24	49	PHE	4.2
32	2a	1030(C)	G	4.1
56	2y	53	G	4.1
41	2j	34	VAL	4.1
1	1A	2174	C	4.1
1	1A	896	A	4.1
34	2c	182	ILE	4.1
56	2y	73	A	4.1
32	2a	1040	U	4.1
56	2y	18	G	4.1
40	2i	128	ARG	4.1
7	2H	4	ILE	4.1
23	2l	68	PRO	4.1
56	2y	69	G	4.1
35	2d	70	ILE	4.1
39	2h	111	ILE	4.1
1	2A	2113	U	4.1
56	1y	56	C	4.1
50	2s	84	GLY	4.1
32	2a	1026	G	4.0
34	2c	155	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
23	11	2	SER	4.0
54	1w	20	U	4.0
29	27	47	ARG	4.0
1	2A	887	A	4.0
1	1A	2113	U	4.0
56	2y	43	C	4.0
1	1A	2121	G	4.0
56	2y	6	G	4.0
1	1A	2117	A	4.0
33	2b	216	SER	4.0
56	2y	26	A	4.0
56	1y	47	U	4.0
40	2i	105	ASP	4.0
45	2n	41	ARG	4.0
32	1a	1030(B)	C	4.0
54	2w	69	G	4.0
56	1y	58	A	4.0
39	2h	9	MET	4.0
45	2n	46	GLU	4.0
34	2c	91	LEU	3.9
33	2b	122	PHE	3.9
20	2Y	65	ALA	3.9
1	1A	2133	G	3.9
1	1A	2118	U	3.9
1	2A	897	C	3.9
53	1v	13	A	3.9
34	2c	82	GLU	3.9
1	1A	2180	U	3.9
56	2y	68	C	3.9
1	1A	278	A	3.9
56	1y	14	A	3.9
38	1g	79	ARG	3.9
35	2d	180	GLY	3.9
56	1y	18	G	3.9
56	1y	57	G	3.9
56	1y	20	U	3.9
3	2D	276	LYS	3.9
44	2m	84	ILE	3.8
56	1y	33	U	3.8
26	24	57	GLU	3.8
33	2b	51	LEU	3.8
34	1c	14	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
35	2d	142	PRO	3.8
7	2H	113	VAL	3.8
33	1b	228	GLY	3.8
56	2y	56	C	3.8
56	1y	64	A	3.8
7	2H	107	VAL	3.8
20	2Y	80	GLY	3.8
41	2j	24	VAL	3.8
56	2y	63	G	3.8
1	1A	2178	C	3.8
45	2n	2	ALA	3.8
52	2u	14	TRP	3.8
48	2q	85	VAL	3.8
1	1A	2154	G	3.8
1	1A	1057	A	3.8
33	2b	19	HIS	3.8
6	2G	3	LEU	3.8
35	2d	68	TYR	3.8
56	1y	61	C	3.8
1	2A	882	G	3.8
1	2A	2144	U	3.8
56	1y	12	U	3.8
56	2y	30	G	3.8
41	2j	88	LEU	3.8
41	2j	67	THR	3.8
33	2b	188	ALA	3.7
43	2l	13	LYS	3.7
23	1l	98	LEU	3.7
1	2A	2801(A)	A	3.7
44	2m	102	ARG	3.7
53	1v	12	A	3.7
1	1A	1064	C	3.7
7	2H	6	ARG	3.7
32	2a	1003	G	3.7
26	14	17	GLY	3.7
54	2w	4	C	3.7
48	2q	11	VAL	3.7
36	2e	99	GLY	3.7
6	2G	29	TRP	3.7
56	2y	71	G	3.7
21	2Z	153	SER	3.7
34	2c	86	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
7	2H	106	THR	3.7
51	2t	9	ASN	3.7
40	2i	13	ALA	3.7
32	2a	1023	G	3.7
35	2d	135	LEU	3.7
35	2d	194	LEU	3.7
39	2h	39	LEU	3.7
1	2A	2139	C	3.7
40	2i	108	VAL	3.7
41	1j	18	ALA	3.7
45	2n	37	PHE	3.7
56	2y	12	U	3.7
1	1A	2158	A	3.7
32	1a	1001(A)	G	3.7
50	2s	68	GLY	3.7
45	2n	53	LEU	3.7
41	2j	68	HIS	3.7
41	2j	96	ILE	3.6
11	2P	109	GLY	3.6
46	2o	66	LEU	3.6
56	1y	73	A	3.6
36	2e	33	VAL	3.6
56	2y	61	C	3.6
34	2c	160	ALA	3.6
1	1A	892	G	3.6
1	2A	881	G	3.6
56	1y	53	G	3.6
12	2Q	19	GLY	3.6
44	2m	87	TYR	3.6
8	2I	81	VAL	3.6
40	2i	7	THR	3.6
56	1y	69	G	3.6
33	1b	118	LEU	3.6
26	24	67	TYR	3.6
1	2A	2114	A	3.6
33	2b	211	ILE	3.6
48	1q	27	PHE	3.6
1	1A	882	G	3.6
41	2j	62	HIS	3.6
56	1y	74	C	3.6
42	1k	25	TYR	3.6
7	2H	125	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
33	2b	93	VAL	3.6
40	2i	75	ASP	3.6
1	2A	2170	A	3.6
33	2b	105	PHE	3.6
52	2u	6	ARG	3.6
40	2i	45	ALA	3.6
40	2i	106	ALA	3.6
44	1m	2	ALA	3.6
56	2y	31	A	3.5
56	2y	45	U	3.5
23	2l	98	LEU	3.5
48	2q	84	LEU	3.5
7	2H	165	ALA	3.5
33	2b	214	ILE	3.5
1	2A	2135	A	3.5
18	1W	112	GLY	3.5
1	2A	2166	G	3.5
35	2d	173	TRP	3.5
39	2h	134	ILE	3.5
1	2A	2167	U	3.5
45	2n	57	ARG	3.5
33	1b	188	ALA	3.5
36	2e	16	THR	3.5
21	2Z	126	VAL	3.5
56	1y	3	C	3.5
38	2g	4	ARG	3.5
40	2i	67	GLY	3.5
40	2i	120	ARG	3.5
46	2o	68	ARG	3.5
49	2r	87	ARG	3.5
56	2y	72	C	3.5
33	2b	37	ASN	3.5
44	2m	4	ILE	3.5
32	1a	1001	A	3.5
56	1y	21	A	3.5
1	1A	2794	C	3.5
33	2b	185	ILE	3.5
56	1y	60	U	3.5
34	1c	15	THR	3.5
40	2i	27	THR	3.5
1	1A	2123	G	3.5
33	2b	139	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	1A	1077	A	3.4
1	1A	1095	A	3.4
32	1a	1030(D)	A	3.4
38	1g	85	TYR	3.4
1	2A	2118	U	3.4
41	2j	36	GLY	3.4
1	2A	2121	G	3.4
1	1A	2175	C	3.4
34	2c	13	GLY	3.4
40	1i	14	VAL	3.4
1	1A	2182	G	3.4
35	2d	190	ASP	3.4
40	2i	62	TYR	3.4
47	1p	38	TYR	3.4
38	2g	41	ARG	3.4
40	2i	65	VAL	3.4
45	2n	25	VAL	3.4
26	24	18	CYS	3.4
36	1e	6	PHE	3.4
1	1A	2101	G	3.4
1	2A	2153	G	3.4
39	2h	112	LEU	3.4
1	2A	2117	A	3.4
1	2A	2161	C	3.4
56	1y	30	G	3.4
40	2i	86	VAL	3.4
34	2c	28	GLN	3.4
45	1n	2	ALA	3.4
56	2y	2	C	3.4
1	1A	1066	U	3.3
1	1A	2122	U	3.3
33	1b	61	LEU	3.3
44	2m	91	ARG	3.3
1	1A	886	C	3.3
1	2A	2129	C	3.3
54	1w	72	C	3.3
1	1A	2166	G	3.3
56	1y	15	G	3.3
43	2l	19	ARG	3.3
11	2P	123	LEU	3.3
40	1i	28	VAL	3.3
1	1A	1075	C	3.3

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Mol	Chain	Res	Type	RSRZ
21	2Z	91	LEU	3.3
48	2q	22	LEU	3.3
56	1y	67	C	3.3
14	2S	5	THR	3.3
1	1A	2168	G	3.3
48	1q	31	LEU	3.3
1	2A	2169	A	3.3
47	1p	7	ALA	3.3
56	1y	51	U	3.3
34	2c	158	GLY	3.3
34	2c	184	TYR	3.3
1	1A	2792	G	3.3
1	2A	2100	G	3.3
1	2A	2181	G	3.3
44	2m	7	VAL	3.3
34	2c	157	ILE	3.3
1	1A	2188	C	3.3
32	2a	1007	C	3.3
33	2b	38	GLY	3.3
53	2v	15	A	3.3
12	2Q	6	ARG	3.3
40	2i	114	TYR	3.3
44	2m	121	LYS	3.3
34	2c	178	LEU	3.2
41	2j	71	LEU	3.2
45	2n	51	GLY	3.2
1	2A	2175	C	3.2
20	2Y	42	VAL	3.2
34	2c	171	GLY	3.2
32	2a	1150	U	3.2
48	2q	59	ILE	3.2
50	2s	69	HIS	3.2
48	2q	89	LEU	3.2
12	2Q	44	ALA	3.2
33	2b	92	TYR	3.2
19	2X	35	THR	3.2
33	2b	118	LEU	3.2
32	1a	1257	U	3.2
6	2G	181	ARG	3.2
56	2y	24	G	3.2
39	2h	93	VAL	3.2
1	1A	2135	A	3.2

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Mol	Chain	Res	Type	RSRZ
32	2a	1286	A	3.2
40	2i	19	LEU	3.2
1	1A	1074	G	3.2
1	1A	2116	G	3.2
12	2Q	109	VAL	3.2
39	2h	65	TYR	3.2
56	1y	22	G	3.2
40	2i	127	LYS	3.2
33	2b	53	ARG	3.2
43	2l	7	ILE	3.2
48	2q	36	ILE	3.2
33	1b	233	SER	3.2
45	2n	33	VAL	3.2
52	2u	8	THR	3.1
1	1A	2142	C	3.1
1	2A	614(B)	G	3.1
1	2A	2168	G	3.1
1	1A	2114	A	3.1
16	2U	17	ILE	3.1
1	1A	2108	C	3.1
46	2o	59	MET	3.1
38	2g	155	ARG	3.1
50	2s	41	VAL	3.1
50	1s	72	GLY	3.1
32	2a	1029	C	3.1
32	1a	1030(C)	G	3.1
32	2a	1030(D)	A	3.1
32	2a	1032	G	3.1
34	1c	179	ARG	3.1
1	2A	2150	U	3.1
40	2i	18	PHE	3.1
1	1A	893	C	3.1
1	1A	2169	A	3.1
34	2c	101	LEU	3.1
41	2j	40	LEU	3.1
46	2o	57	LEU	3.1
1	1A	2136	C	3.1
1	1A	2803	C	3.1
46	2o	17	ARG	3.1
29	27	46	VAL	3.1
45	2n	40	CYS	3.1
1	1A	1078	U	3.1

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Mol	Chain	Res	Type	RSRZ
11	2P	91	PHE	3.1
20	2Y	38	ILE	3.1
32	1a	841	U	3.1
38	2g	85	TYR	3.1
48	2q	92	ARG	3.1
1	1A	1076	C	3.1
21	2Z	166	SER	3.1
35	2d	162	LEU	3.1
39	2h	36	LEU	3.1
40	2i	103	THR	3.1
41	2j	8	LEU	3.1
56	2y	76	A	3.0
1	1A	895	U	3.0
1	1A	1176	G	3.0
1	2A	2152	G	3.0
49	2r	65	ILE	3.0
35	1d	111	ALA	3.0
41	2j	27	ALA	3.0
33	2b	229	VAL	3.0
1	2A	229	A	3.0
41	2j	74	ILE	3.0
1	1A	2153	G	3.0
1	1A	2187	G	3.0
34	2c	15	THR	3.0
40	2i	102	LEU	3.0
40	2i	123	PRO	3.0
1	1A	229	A	3.0
1	1A	2134	A	3.0
1	2A	2119	A	3.0
41	2j	69	ASN	3.0
1	2A	2191	G	3.0
47	1p	27	LYS	3.0
51	2t	12	ALA	3.0
38	2g	105	VAL	3.0
45	2n	14	PRO	3.0
56	1y	4	C	3.0
21	2Z	106	GLY	3.0
12	2Q	113	GLN	3.0
44	2m	23	TYR	3.0
51	2t	8	ARG	3.0
51	1t	19	SER	3.0
12	2Q	2	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
43	2l	60	LEU	3.0
44	2m	96	LEU	3.0
51	1t	20	LEU	3.0
1	1A	879	G	3.0
1	2A	2182	G	3.0
39	2h	67	PRO	3.0
50	2s	76	PRO	3.0
42	2k	109	VAL	3.0
35	2d	6	GLY	3.0
1	2A	2177	C	3.0
12	2Q	66	ILE	3.0
29	17	47	ARG	3.0
38	2g	42	ILE	3.0
40	2i	121	ARG	3.0
45	2n	36	PHE	3.0
39	2h	4	ASP	3.0
34	2c	48	TYR	3.0
34	2c	193	TYR	3.0
35	2d	186	LEU	3.0
36	2e	62	ALA	3.0
39	2h	133	LEU	3.0
8	2I	145	VAL	3.0
39	2h	26	VAL	3.0
56	1y	27	G	3.0
56	1y	63	G	3.0
56	2y	19	G	3.0
1	2A	2132	U	3.0
56	1y	11	C	3.0
8	2I	49	ALA	3.0
34	2c	33	LEU	3.0
50	2s	71	LEU	3.0
33	2b	152	PHE	2.9
32	1a	1030(A)	G	2.9
32	1a	1032	G	2.9
7	2H	105	LEU	2.9
35	2d	188	LEU	2.9
38	2g	25	ALA	2.9
36	2e	85	GLY	2.9
38	1g	84	ASN	2.9
44	1m	89	GLY	2.9
34	2c	22	TRP	2.9
39	1h	26	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
7	2H	123	PHE	2.9
38	2g	7	ALA	2.9
44	2m	97	PRO	2.9
20	2Y	45	VAL	2.9
33	2b	201	ILE	2.9
36	2e	81	GLU	2.9
39	2h	35	ILE	2.9
34	2c	145	GLY	2.9
48	2q	33	GLY	2.9
1	1A	2179	C	2.9
33	2b	220	ASP	2.9
45	2n	54	PRO	2.9
32	2a	998	G	2.9
20	2Y	24	VAL	2.9
41	2j	9	ARG	2.9
40	2i	87	GLN	2.9
53	2v	14	A	2.9
38	2g	30	ILE	2.9
46	2o	5	LYS	2.9
39	2h	124	ALA	2.9
51	1t	12	ALA	2.9
1	2A	2136	C	2.9
40	2i	66	ARG	2.9
56	1y	25	C	2.9
9	2N	9	VAL	2.9
22	20	23	VAL	2.9
27	15	60	VAL	2.9
33	2b	17	PHE	2.9
40	2i	77	ILE	2.9
41	2j	98	ILE	2.9
7	2H	112	PRO	2.9
51	2t	72	LEU	2.9
46	1o	89	GLY	2.9
32	2a	1002	G	2.9
32	2a	1024	G	2.9
56	2y	27	G	2.9
39	2h	122	ARG	2.9
1	1A	2139	C	2.8
22	20	42	GLY	2.8
48	2q	23	VAL	2.8
32	2a	1257	U	2.8
40	2i	124	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
34	2c	146	ALA	2.8
32	1a	161	A	2.8
52	1u	14	TRP	2.8
35	2d	106	TYR	2.8
50	2s	35	SER	2.8
45	1n	56	VAL	2.8
33	1b	222	ILE	2.8
48	1q	36	ILE	2.8
51	1t	72	LEU	2.8
33	1b	36	ARG	2.8
1	2A	895	U	2.8
35	2d	146	ILE	2.8
38	2g	120	ILE	2.8
56	1y	59	U	2.8
21	2Z	156	LYS	2.8
35	2d	196	LEU	2.8
45	2n	29	ARG	2.8
50	2s	72	GLY	2.8
40	1i	126	SER	2.8
1	2A	2157	G	2.8
40	2i	5	TYR	2.8
1	2A	2122	U	2.8
20	2Y	44	ILE	2.8
20	2Y	61	ILE	2.8
39	2h	6	ILE	2.8
44	2m	42	ALA	2.8
50	2s	78	ARG	2.8
56	1y	48	C	2.8
43	2l	27	LEU	2.8
40	1i	100	GLY	2.8
29	17	1	MET	2.8
26	14	63	TYR	2.8
47	2p	58	TYR	2.8
1	2A	2159	G	2.8
1	2A	2190	G	2.8
32	1a	1003	G	2.8
54	2w	44	G	2.8
56	1y	28	G	2.8
39	2h	38	ILE	2.8
33	2b	218	ALA	2.8
37	1f	16	GLN	2.8
54	1w	67	C	2.8

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Mol	Chain	Res	Type	RSRZ
20	2Y	3	VAL	2.8
29	17	46	VAL	2.8
41	2j	89	ASP	2.8
53	2v	13	A	2.8
9	2N	69	GLN	2.8
33	2b	33	TYR	2.8
6	1G	77	ILE	2.8
11	2P	58	THR	2.8
21	2Z	147	GLY	2.8
33	2b	168	THR	2.8
1	1A	2104	G	2.8
32	2a	1021	G	2.8
44	2m	92	HIS	2.8
1	1A	890	A	2.7
1	2A	2173	A	2.7
32	1a	1035	A	2.7
35	2d	20	TYR	2.7
36	2e	146	ALA	2.7
48	2q	90	ILE	2.7
1	1A	2127	G	2.7
41	2j	39	PRO	2.7
9	2N	140	VAL	2.7
31	29	29	ASN	2.7
39	1h	112	LEU	2.7
42	1k	126	ARG	2.7
45	2n	16	PHE	2.7
7	2H	159	GLU	2.7
1	2A	2148	G	2.7
56	1y	10	G	2.7
36	2e	32	VAL	2.7
26	24	55	ARG	2.7
1	2A	2180	U	2.7
45	2n	22	THR	2.7
12	2Q	17	LEU	2.7
1	1A	2107	C	2.7
44	2m	99	ARG	2.7
1	1A	2155	G	2.7
32	2a	1061	G	2.7
14	2S	36	TYR	2.7
36	2e	31	LEU	2.7
33	2b	16	HIS	2.7
1	1A	1072	C	2.7

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Mol	Chain	Res	Type	RSRZ
56	2y	41	C	2.7
6	2G	161	THR	2.7
42	1k	15	ALA	2.7
26	24	42	PHE	2.7
34	1c	94	LEU	2.7
47	1p	60	LEU	2.7
51	1t	63	ILE	2.7
48	2q	81	ARG	2.7
52	2u	24	ARG	2.7
32	2a	1248	A	2.7
1	2A	2140	C	2.7
29	27	45	ALA	2.7
32	2a	1028	C	2.7
39	2h	33	GLU	2.7
56	2y	4	C	2.7
34	2c	94	LEU	2.7
39	1h	133	LEU	2.7
1	1A	2100	G	2.7
1	1A	2793	G	2.7
32	2a	1224	G	2.7
41	2j	25	GLU	2.6
43	2l	18	VAL	2.6
3	2D	38	LYS	2.6
20	2Y	54	LYS	2.6
32	1a	204	U	2.6
48	2q	31	LEU	2.6
7	2H	46	GLU	2.6
1	2A	2124	G	2.6
32	2a	1220	G	2.6
51	1t	80	ARG	2.6
21	1Z	166	SER	2.6
40	2i	28	VAL	2.6
1	1A	1067	A	2.6
1	2A	1847	A	2.6
21	2Z	151	HIS	2.6
34	2c	177	THR	2.6
49	2r	60	ALA	2.6
56	2y	7	A	2.6
33	2b	155	LEU	2.6
48	2q	8	GLY	2.6
1	1A	2804	C	2.6
1	2A	2188	C	2.6

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Mol	Chain	Res	Type	RSRZ
40	2i	110	GLU	2.6
48	1q	28	PRO	2.6
56	1y	72	C	2.6
45	2n	4	LYS	2.6
1	1A	2152	G	2.6
1	1A	2165	G	2.6
1	1A	271(K)	U	2.6
1	1A	1026	U	2.6
32	1a	1446	U	2.6
45	2n	52	GLN	2.6
50	2s	12	ASP	2.6
26	24	68	ARG	2.6
45	2n	43	CYS	2.6
48	2q	91	ARG	2.6
32	1a	999	C	2.6
8	2I	46	ALA	2.6
9	2N	27	ALA	2.6
33	2b	71	VAL	2.6
36	2e	72	GLN	2.6
48	2q	35	VAL	2.6
50	2s	48	THR	2.6
1	1A	2151	G	2.6
1	2A	2120	G	2.6
1	2A	2149	G	2.6
20	2Y	63	LYS	2.6
46	2o	65	ARG	2.6
56	2y	50	U	2.6
19	2X	89	ILE	2.6
33	1b	214	ILE	2.6
1	1A	2170	A	2.6
32	2a	263	A	2.6
50	2s	66	MET	2.6
47	2p	38	TYR	2.6
33	2b	233	SER	2.6
34	2c	61	ALA	2.6
40	2i	53	VAL	2.6
45	2n	12	ARG	2.6
7	2H	103	LEU	2.6
41	1j	16	LEU	2.6
32	2a	1256	A	2.6
33	2b	171	ALA	2.6
40	2i	122	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
25	23	2	PRO	2.6
40	2i	50	LEU	2.6
54	2w	45	U	2.6
1	2A	2106	G	2.6
54	2w	5	G	2.6
36	2e	17	ALA	2.5
42	1k	69	ALA	2.5
41	2j	44	VAL	2.5
45	1n	14	PRO	2.5
47	2p	51	VAL	2.5
8	2l	38	LEU	2.5
38	2g	99	LEU	2.5
6	2G	140	ILE	2.5
8	2I	4	ILE	2.5
39	2h	86	ILE	2.5
41	2j	47	PHE	2.5
12	2Q	5	ARG	2.5
40	2i	9	ARG	2.5
7	2H	111	HIS	2.5
1	2A	878	A	2.5
29	17	45	ALA	2.5
31	29	16	VAL	2.5
32	1a	1029	C	2.5
32	2a	1149	C	2.5
41	2j	90	LEU	2.5
32	2a	1446	U	2.5
7	2H	100	GLY	2.5
43	2l	14	GLY	2.5
38	2g	83	ALA	2.5
43	2l	64	TYR	2.5
48	2q	44	ALA	2.5
43	1l	18	VAL	2.5
32	1a	163	C	2.5
34	2c	159	GLY	2.5
33	2b	28	PHE	2.5
38	2g	26	PHE	2.5
40	2i	63	ILE	2.5
46	2o	15	PHE	2.5
48	2q	27	PHE	2.5
51	1t	18	GLN	2.5
34	2c	190	ARG	2.5
38	2g	6	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
44	2m	64	TRP	2.5
32	2a	1041	A	2.5
56	2y	58	A	2.5
1	1A	2897	U	2.5
54	2w	67	C	2.5
56	2y	48	C	2.5
1	1A	2148	G	2.5
1	2A	2151	G	2.5
41	2j	6	ILE	2.5
21	1Z	168	GLU	2.5
3	2D	77	ALA	2.5
41	2j	12	ASP	2.5
45	2n	61	TRP	2.5
11	2P	59	LEU	2.5
11	2P	110	TYR	2.5
44	1m	87	TYR	2.5
47	1p	49	LEU	2.5
49	1r	85	LEU	2.5
1	2A	6	A	2.5
32	2a	1001	A	2.5
56	1y	66	U	2.5
35	2d	158	ILE	2.5
39	2h	13	ILE	2.5
48	1q	99	SER	2.5
1	2A	2162	G	2.5
36	1e	132	ALA	2.5
38	2g	46	ALA	2.5
34	2c	96	GLY	2.5
38	1g	82	GLY	2.5
3	2D	182	LEU	2.5
20	2Y	106	LEU	2.5
30	28	61	LEU	2.5
39	1h	118	VAL	2.5
44	2m	60	VAL	2.5
45	2n	44	LEU	2.5
51	2t	16	HIS	2.5
52	2u	22	ARG	2.5
22	20	45	PHE	2.5
32	2a	1157	A	2.5
36	2e	80	ILE	2.5
51	1t	14	LYS	2.5
53	1v	14	A	2.5

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Mol	Chain	Res	Type	RSRZ
32	1a	1024	G	2.5
46	2o	61	GLY	2.5
51	2t	26	ASN	2.5
8	2I	60	GLU	2.5
35	2d	104	VAL	2.4
46	2o	60	VAL	2.4
54	2w	47	U	2.4
36	1e	10	MET	2.4
21	1Z	169	GLU	2.4
51	1t	9	ASN	2.4
54	1w	4	C	2.4
56	2y	25	C	2.4
3	1D	2	ALA	2.4
23	2l	69	LYS	2.4
44	2m	103	THR	2.4
1	1A	1063	G	2.4
32	2a	1202	G	2.4
56	1y	6	G	2.4
11	2P	101	VAL	2.4
48	2q	73	VAL	2.4
47	1p	9	PHE	2.4
50	2s	62	ILE	2.4
7	2H	161	GLY	2.4
8	2I	74	ASN	2.4
40	2i	73	GLN	2.4
50	2s	82	GLY	2.4
38	1g	153	HIS	2.4
52	1u	8	THR	2.4
7	2H	16	SER	2.4
1	1A	2125	G	2.4
11	2P	65	ARG	2.4
47	2p	59	TRP	2.4
52	2u	9	ARG	2.4
7	2H	36	PRO	2.4
1	1A	2138	C	2.4
1	1A	2177	C	2.4
56	2y	67	C	2.4
3	2D	275	LYS	2.4
6	2G	37	VAL	2.4
34	1c	64	VAL	2.4
39	2h	79	VAL	2.4
44	2m	117	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
15	2T	48	ILE	2.4
20	2Y	75	ILE	2.4
56	1y	52	G	2.4
36	1e	95	ALA	2.4
6	2G	166	ASP	2.4
35	1d	194	LEU	2.4
35	2d	141	ARG	2.4
56	1y	49	C	2.4
8	2I	144	VAL	2.4
45	2n	18	VAL	2.4
48	2q	10	VAL	2.4
50	1s	58	VAL	2.4
44	2m	12	ASN	2.4
56	2y	47	U	2.4
6	1G	146	TYR	2.4
15	2T	100	TYR	2.4
34	1c	124	ILE	2.4
45	2n	49	HIS	2.4
43	2l	56	ALA	2.4
51	1t	32	ALA	2.4
1	2A	2156	G	2.4
34	1c	87	LEU	2.4
1	2A	2134	A	2.4
10	2O	102	VAL	2.4
32	1a	1027	C	2.4
40	2i	29	ASN	2.4
40	2i	98	PRO	2.4
51	1t	76	ALA	2.4
9	2N	73	THR	2.4
42	2k	87	THR	2.4
9	2N	10	GLU	2.4
39	2h	138	TRP	2.4
21	2Z	125	LEU	2.4
56	1y	65	G	2.3
47	1p	37	GLY	2.3
39	2h	19	VAL	2.3
1	2A	652(B)	A	2.3
1	2A	2158	A	2.3
53	2v	23	A	2.3
41	2j	77	PRO	2.3
28	26	28	ARG	2.3
45	2n	26	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
36	2e	138	ALA	2.3
12	2Q	33	GLY	2.3
38	2g	22	LEU	2.3
48	2q	94	ASN	2.3
1	2A	2807	G	2.3
20	2Y	7	VAL	2.3
20	2Y	30	VAL	2.3
32	1a	1000	U	2.3
32	1a	1033	G	2.3
35	2d	178	VAL	2.3
38	1g	155	ARG	2.3
41	2j	91	PRO	2.3
51	2t	83	ARG	2.3
52	1u	15	ARG	2.3
1	1A	2171	A	2.3
4	2E	134	ILE	2.3
32	1a	162	A	2.3
50	1s	31	ILE	2.3
40	2i	4	TYR	2.3
30	28	17	THR	2.3
33	2b	210	SER	2.3
36	1e	16	THR	2.3
3	1D	223	GLY	2.3
7	1H	7	LEU	2.3
6	1G	38	VAL	2.3
34	2c	17	ASP	2.3
39	2h	61	VAL	2.3
41	2j	73	ASP	2.3
7	2H	25	LYS	2.3
29	17	48	LYS	2.3
55	2x	47	U	2.3
13	2R	34	ILE	2.3
1	2A	898	C	2.3
32	2a	1154	G	2.3
36	2e	84	PHE	2.3
32	1a	1286	A	2.3
34	2c	65	ALA	2.3
56	1y	31	A	2.3
19	2X	66	LEU	2.3
35	2d	187	ARG	2.3
44	1m	96	LEU	2.3
8	2I	20	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
41	2j	21	GLN	2.3
1	2A	2189	U	2.3
19	2X	61	GLY	2.3
20	2Y	25	GLY	2.3
1	1A	2184	G	2.3
21	2Z	8	TYR	2.3
32	2a	80	G	2.3
32	2a	1006	C	2.3
44	1m	30	ALA	2.3
21	2Z	24	LEU	2.3
41	1j	85	LEU	2.3
13	2R	39	PRO	2.3
16	2U	2	PRO	2.3
25	23	56	VAL	2.3
1	1A	2167	U	2.3
1	2A	1026	U	2.3
7	2H	51	ARG	2.3
15	1T	108	ARG	2.3
21	1Z	133	ILE	2.3
26	24	62	ARG	2.3
34	1c	182	ILE	2.3
34	2c	53	ALA	2.3
41	2j	87	THR	2.3
1	2A	2116	G	2.3
26	24	48	ARG	2.3
41	2j	29	ARG	2.3
7	2H	30	LYS	2.3
30	28	29	LYS	2.3
35	2d	175	SER	2.3
40	2i	24	GLY	2.3
41	1j	10	GLY	2.3
33	2b	120	ALA	2.3
43	2l	51	ALA	2.3
38	1g	154	TYR	2.3
32	2a	978	A	2.2
4	2E	196	VAL	2.2
42	2k	117	ASN	2.2
32	2a	204	U	2.2
32	2a	1025	U	2.2
17	2V	73	SER	2.2
21	1Z	164	ALA	2.2
37	2f	81	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
3	2D	161	THR	2.2
48	1q	7	THR	2.2
11	1P	108	LYS	2.2
21	2Z	38	TYR	2.2
26	24	32	TYR	2.2
33	2b	64	ARG	2.2
42	1k	66	LEU	2.2
44	2m	90	LEU	2.2
1	1A	894	C	2.2
1	1A	2183	C	2.2
12	2Q	23	GLY	2.2
40	2i	57	GLY	2.2
44	1m	74	VAL	2.2
39	1h	87	SER	2.2
1	2A	2319	G	2.2
32	1a	1034	G	2.2
56	1y	29	G	2.2
33	2b	39	ILE	2.2
34	1c	8	ILE	2.2
34	1c	77	ILE	2.2
35	1d	147	ALA	2.2
27	25	29	THR	2.2
41	1j	47	PHE	2.2
12	1Q	6	ARG	2.2
45	2n	3	ARG	2.2
6	1G	139	LEU	2.2
7	2H	71	LEU	2.2
8	2I	89	TYR	2.2
35	1d	4	TYR	2.2
45	2n	55	GLY	2.2
51	1t	47	GLY	2.2
1	1A	2164	C	2.2
1	1A	2185	C	2.2
1	2A	2137	C	2.2
42	2k	114	VAL	2.2
32	2a	1250	A	2.2
38	1g	6	ARG	2.2
44	2m	94	ARG	2.2
35	2d	64	LEU	2.2
20	2Y	29	GLU	2.2
21	2Z	154	ASP	2.2
6	2G	182	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
34	2c	23	TYR	2.2
47	1p	17	TYR	2.2
32	1a	1532	U	2.2
38	1g	21	VAL	2.2
1	1A	878	A	2.2
7	2H	122	THR	2.2
32	2a	1287	A	2.2
40	1i	119	ALA	2.2
16	2U	32	PHE	2.2
43	1l	16	GLU	2.2
50	2s	27	GLU	2.2
6	2G	19	LEU	2.2
35	1d	138	TYR	2.2
45	1n	61	TRP	2.2
23	2l	8	SER	2.2
1	1A	898	C	2.2
32	2a	1249	C	2.2
32	2a	1452	C	2.2
36	1e	17	ALA	2.2
42	1k	89	ALA	2.2
51	2t	78	ALA	2.2
26	14	49	PHE	2.2
35	2d	184	LYS	2.2
39	2h	44	PHE	2.2
50	2s	28	LYS	2.2
11	2P	45	LEU	2.2
46	2o	89	GLY	2.2
34	1c	83	ARG	2.2
51	1t	83	ARG	2.2
11	1P	149	GLU	2.2
52	2u	21	TYR	2.2
1	1A	2102	U	2.2
21	2Z	165	VAL	2.2
36	2e	20	GLN	2.2
47	2p	20	VAL	2.2
50	1s	60	VAL	2.2
14	2S	6	ALA	2.2
39	2h	120	THR	2.2
48	2q	65	ILE	2.2
34	2c	185	GLY	2.2
33	2b	131	PRO	2.2
36	2e	24	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
38	2g	5	ARG	2.2
1	2A	2126	A	2.2
40	2i	79	LEU	2.2
35	2d	31	CYS	2.2
1	1A	1068	G	2.1
1	2A	1719	G	2.1
1	2A	2104	G	2.1
7	2H	141	VAL	2.1
32	1a	1025	U	2.1
33	2b	177	ALA	2.1
42	2k	23	ALA	2.1
26	14	45	GLY	2.1
35	2d	16	GLY	2.1
36	2e	64	ARG	2.1
38	2g	27	ILE	2.1
45	1n	13	THR	2.1
1	2A	2108	C	2.1
32	1a	1028	C	2.1
35	2d	120	LEU	2.1
33	2b	95	GLN	2.1
33	2b	195	ASP	2.1
39	2h	62	TYR	2.1
1	1A	1094	U	2.1
5	2F	36	VAL	2.1
16	1U	8	VAL	2.1
7	2H	18	GLU	2.1
17	2V	63	GLY	2.1
19	2X	10	ALA	2.1
21	2Z	145	GLU	2.1
26	24	54	GLY	2.1
33	1b	123	ALA	2.1
33	2b	227	GLY	2.1
47	1p	24	ALA	2.1
17	2V	92	THR	2.1
36	2e	120	THR	2.1
1	2A	2805	G	2.1
32	1a	1026	G	2.1
32	2a	1392	G	2.1
39	2h	83	ILE	2.1
46	2o	18	PHE	2.1
50	2s	74	PHE	2.1
4	1E	195	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
44	1m	90	LEU	2.1
48	2q	26	GLN	2.1
1	1A	2103	C	2.1
1	2A	2896	C	2.1
29	17	23	ARG	2.1
44	2m	80	ARG	2.1
36	1e	121	LYS	2.1
50	2s	54	GLY	2.1
1	1A	1175	U	2.1
41	1j	94	VAL	2.1
44	2m	118	ALA	2.1
46	2o	16	ALA	2.1
56	2y	51	U	2.1
56	2y	60	U	2.1
50	2s	63	THR	2.1
3	2D	155	LEU	2.1
5	2F	24	LEU	2.1
20	2Y	31	LEU	2.1
51	2t	24	LEU	2.1
1	2A	2165	G	2.1
1	1A	2896	C	2.1
38	2g	123	GLU	2.1
7	2H	13	LYS	2.1
33	2b	66	GLY	2.1
9	2N	72	TYR	2.1
33	1b	164	VAL	2.1
34	2c	180	ALA	2.1
35	2d	140	VAL	2.1
36	2e	105	VAL	2.1
36	1e	135	THR	2.1
39	1h	35	ILE	2.1
8	2I	82	ARG	2.1
33	2b	170	GLU	2.1
34	2c	175	LEU	2.1
35	2d	11	LEU	2.1
35	2d	110	PHE	2.1
42	2k	96	ARG	2.1
38	2g	33	ASP	2.1
51	1t	74	LYS	2.1
11	2P	66	GLY	2.1
33	2b	228	GLY	2.1
34	2c	74	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
11	2P	103	ALA	2.1
33	1b	225	ALA	2.1
34	1c	180	ALA	2.1
1	2A	2171	A	2.1
35	1d	20	TYR	2.1
41	2j	41	PRO	2.1
50	2s	45	VAL	2.1
52	1u	21	TYR	2.1
54	2w	73	A	2.1
21	2Z	171	ILE	2.1
11	2P	115	LEU	2.1
33	1b	10	LEU	2.1
34	2c	34	LEU	2.1
35	1d	113	SER	2.1
39	2h	87	SER	2.1
26	14	54	GLY	2.1
11	2P	149	GLU	2.1
20	2Y	5	MET	2.1
32	1a	1037	C	2.1
1	1A	1099	G	2.1
1	1A	2186	G	2.1
1	1A	2833	G	2.1
38	1g	4	ARG	2.1
38	2g	39	ALA	2.1
50	2s	37	ARG	2.1
51	2t	86	ARG	2.1
21	2Z	161	VAL	2.1
34	1c	207	VAL	2.1
43	2l	39	VAL	2.1
16	2U	24	TYR	2.1
32	2a	1092	A	2.1
51	1t	16	HIS	2.1
8	2I	44	LEU	2.1
26	24	59	PHE	2.1
48	2q	39	SER	2.1
9	1N	139	GLU	2.1
42	2k	46	GLY	2.1
44	2m	100	GLY	2.1
45	2n	31	ARG	2.1
1	2A	894	C	2.0
4	1E	28	ALA	2.0
18	2W	89	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
25	23	12	PRO	2.0
32	2a	1284	C	2.0
36	1e	138	ALA	2.0
1	1A	1065	U	2.0
8	2I	86	THR	2.0
33	1b	230	VAL	2.0
47	1p	62	VAL	2.0
48	2q	21	VAL	2.0
50	2s	51	VAL	2.0
6	2G	11	TYR	2.0
6	2G	146	TYR	2.0
18	2W	38	TYR	2.0
35	2d	27	TYR	2.0
54	1w	44	G	2.0
1	2A	890	A	2.0
1	2A	899	A	2.0
5	2F	202	PHE	2.0
27	25	59	GLU	2.0
39	2h	45	ILE	2.0
48	2q	12	SER	2.0
35	2d	19	LEU	2.0
40	1i	31	GLN	2.0
53	2v	24	A	2.0
56	1y	76	A	2.0
40	2i	112	LYS	2.0
6	2G	136	ARG	2.0
38	2g	31	MET	2.0
23	11	24	ALA	2.0
42	1k	60	ALA	2.0
1	2A	2794	C	2.0
5	2F	37	VAL	2.0
17	2V	33	VAL	2.0
37	2f	90	VAL	2.0
40	1i	109	VAL	2.0
49	1r	86	VAL	2.0
6	2G	138	GLN	2.0
12	2Q	18	LYS	2.0
18	2W	101	SER	2.0
21	2Z	57	ILE	2.0
23	21	67	ILE	2.0
15	1T	111	ARG	2.0
21	2Z	59	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
36	2e	118	ILE	2.0
38	2g	78	ARG	2.0
48	2q	53	LEU	2.0
32	2a	1370	G	2.0
26	14	51	ASP	2.0
26	14	57	GLU	2.0
41	2j	64	GLU	2.0
22	20	33	ALA	2.0
40	1i	113	LYS	2.0
41	2j	32	ALA	2.0
44	2m	72	ALA	2.0
46	2o	4	THR	2.0
21	1Z	165	VAL	2.0
34	1c	68	VAL	2.0
34	2c	83	ARG	2.0
40	2i	10	ARG	2.0
40	2i	42	ARG	2.0
32	2a	1115	C	2.0
6	2G	152	LEU	2.0
8	1I	35	LEU	2.0
6	1G	80	PHE	2.0
38	2g	146	GLU	2.0
1	1A	2801(A)	A	2.0
32	2a	216	G	2.0
32	2a	1005	A	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	MIA	2y	37	22/30	0.57	0.47	76,85,95,115	0
56	PSU	2y	55	20/21	0.60	0.41	76,83,96,102	0
56	PSU	1y	55	20/21	0.68	0.40	79,86,94,95	0
56	7MG	2y	46	24/25	0.68	0.38	80,91,96,105	0
56	4SU	2y	8	20/21	0.72	0.29	81,89,99,105	0
56	PSU	2y	39	20/21	0.74	0.49	75,85,94,103	0
56	PSU	2y	32	20/21	0.74	0.42	68,85,93,104	0
56	MIA	1y	37	22/30	0.76	0.36	72,78,92,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	7MG	1y	46	24/25	0.77	0.27	77,85,94,100	0
54	7MG	2w	46	24/25	0.77	0.21	67,75,92,102	0
56	5MU	1y	54	21/22	0.77	0.31	77,82,87,93	0
56	PSU	1y	32	20/21	0.78	0.34	74,80,92,102	0
56	PSU	1y	39	20/21	0.78	0.33	68,82,89,89	0
56	5MU	2y	54	21/22	0.78	0.42	79,83,91,106	0
56	4SU	1y	8	20/21	0.78	0.27	79,86,91,104	0
54	4SU	2w	8	20/21	0.81	0.19	72,78,91,92	0
54	7MG	1w	46	24/25	0.82	0.17	61,70,88,106	0
43	0TD	2l	92	10/11	0.85	0.17	50,55,64,82	0
54	PSU	2w	55	20/21	0.87	0.15	66,73,79,85	0
54	5MU	2w	54	21/22	0.88	0.16	61,67,76,78	0
54	4SU	1w	8	20/21	0.88	0.17	66,73,81,84	0
54	PSU	2w	32	20/21	0.89	0.28	63,70,75,76	0
32	2MG	2a	1207	24/25	0.90	0.20	68,72,77,82	0
32	M2G	2a	966	25/26	0.90	0.23	46,55,71,79	0
55	PSU	2x	55	20/21	0.90	0.18	59,66,75,75	0
55	4SU	2x	8	20/21	0.90	0.15	62,65,70,70	0
55	5MU	2x	54	21/22	0.91	0.23	65,68,74,85	0
54	MIA	2w	37	25/30	0.92	0.24	50,63,71,88	0
54	PSU	1w	55	20/21	0.92	0.17	53,61,67,69	0
43	0TD	1l	92	10/11	0.92	0.22	39,45,47,55	0
54	PSU	2w	39	20/21	0.93	0.24	64,68,73,73	0
55	PSU	1x	55	20/21	0.93	0.18	44,50,59,61	0
55	4SU	1x	8	20/21	0.93	0.17	40,50,58,59	0
55	5MU	1x	54	21/22	0.93	0.17	50,58,60,61	0
32	7MG	2a	527	24/25	0.93	0.17	44,58,64,65	0
32	PSU	2a	516	20/21	0.93	0.20	55,61,69,69	0
1	PSU	2A	1917	20/21	0.94	0.17	42,51,56,56	0
32	5MC	2a	967	21/22	0.94	0.19	55,61,65,69	0
32	5MC	2a	1404	21/22	0.94	0.18	41,54,57,60	0
54	PSU	1w	32	20/21	0.94	0.17	43,49,58,59	0
1	5MU	2A	1915	21/22	0.94	0.17	46,55,60,61	0
1	4OC	2A	1920	21/23	0.94	0.17	44,51,54,57	0
32	UR3	2a	1498	21/22	0.95	0.21	41,50,54,56	0
54	5MU	1w	54	21/22	0.95	0.17	40,50,58,61	0
54	MIA	1w	37	29/30	0.95	0.20	32,42,59,72	0
32	2MG	1a	1207	24/25	0.95	0.16	46,54,57,62	0
1	5MU	1A	1915	21/22	0.95	0.20	31,40,48,52	0
1	5MC	2A	1962	21/22	0.96	0.18	31,42,49,56	0
32	7MG	1a	527	24/25	0.96	0.18	33,41,49,51	0
32	5MC	1a	1404	21/22	0.96	0.19	29,37,39,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	5MC	2x	32	21/22	0.96	0.20	59,63,67,72	0
32	4OC	2a	1402	22/23	0.96	0.18	42,53,58,58	0
1	5MC	2A	1942	21/22	0.96	0.18	40,48,52,58	0
32	5MC	2a	1400	21/22	0.96	0.28	48,59,63,64	0
55	31H	1x	76	32/33	0.96	0.23	13,21,26,33	10
32	4OC	1a	1402	22/23	0.96	0.16	37,43,46,48	0
32	MA6	2a	1519	24/25	0.96	0.23	48,56,59,60	0
55	31H	2x	76	32/33	0.96	0.20	24,34,44,48	0
1	5MU	2A	1939	21/22	0.96	0.19	28,33,36,41	0
54	PSU	1w	39	20/21	0.96	0.21	32,51,57,60	0
32	5MC	1a	1400	21/22	0.96	0.19	28,39,43,51	0
1	PSU	1A	1917	20/21	0.96	0.20	29,44,50,51	0
54	F3N	2w	76	33/34	0.96	0.21	30,35,41,42	0
32	M2G	1a	966	25/26	0.96	0.21	34,39,42,47	0
32	5MC	2a	1407	21/22	0.96	0.20	46,52,56,58	0
1	PSU	1A	1911	20/21	0.96	0.17	39,42,46,50	0
55	5MC	1x	32	21/22	0.96	0.18	39,43,50,60	0
32	5MC	1a	967	21/22	0.96	0.18	35,42,46,49	0
32	PSU	1a	516	20/21	0.96	0.17	40,48,54,54	0
1	PSU	2A	1911	20/21	0.96	0.18	41,53,60,63	0
32	5MC	1a	1407	21/22	0.96	0.18	23,37,40,43	0
1	OMG	2A	2251	24/25	0.97	0.20	27,34,37,41	0
54	F3N	1w	76	33/34	0.97	0.23	15,20,23,25	0
1	5MU	1A	1939	21/22	0.97	0.22	17,23,29,30	0
1	PSU	2A	2605	20/21	0.97	0.20	23,32,38,39	0
32	MA6	2a	1518	24/25	0.97	0.22	49,54,59,63	0
1	2MA	1A	2503	23/24	0.97	0.22	10,17,23,28	0
1	5MC	1A	1942	21/22	0.97	0.17	31,40,45,49	0
32	MA6	1a	1519	24/25	0.97	0.21	29,36,39,44	0
1	2MU	2A	2552	21/23	0.97	0.23	32,38,43,44	0
1	5MC	1A	1962	21/22	0.98	0.20	18,25,34,37	0
1	2MA	2A	2503	23/24	0.98	0.20	26,29,33,38	0
1	2MU	1A	2552	21/23	0.98	0.20	16,25,29,32	0
1	OMG	1A	2251	24/25	0.98	0.21	15,23,26,28	0
1	PSU	1A	2605	20/21	0.98	0.20	17,22,26,27	0
1	4OC	1A	1920	21/23	0.98	0.18	35,40,42,43	0
32	MA6	1a	1518	24/25	0.98	0.21	30,36,40,40	0
32	UR3	1a	1498	21/22	0.98	0.18	26,31,37,38	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	2A	3917	1/1	0.17	0.47	77,77,77,77	0
57	MG	1A	4141	1/1	0.30	0.20	48,48,48,48	0
57	MG	1A	4227	1/1	0.33	0.21	65,65,65,65	0
57	MG	2a	3062	1/1	0.34	0.20	79,79,79,79	0
57	MG	1a	3225	1/1	0.38	0.09	63,63,63,63	0
57	MG	1A	4212	1/1	0.40	0.23	55,55,55,55	0
57	MG	2a	3183	1/1	0.43	0.21	72,72,72,72	0
57	MG	1a	3226	1/1	0.45	0.20	68,68,68,68	0
57	MG	2a	3064	1/1	0.45	0.37	65,65,65,65	0
57	MG	1A	4086	1/1	0.47	0.23	70,70,70,70	0
57	MG	2a	3116	1/1	0.48	0.32	63,63,63,63	0
57	MG	2A	3202	1/1	0.48	0.25	62,62,62,62	0
57	MG	1A	3330	1/1	0.48	0.22	63,63,63,63	0
57	MG	2A	3882	1/1	0.48	0.16	51,51,51,51	0
57	MG	1A	3425	1/1	0.49	0.38	55,55,55,55	0
57	MG	2A	3186	1/1	0.50	0.18	50,50,50,50	0
57	MG	1a	3074	1/1	0.51	0.20	60,60,60,60	0
57	MG	2A	3813	1/1	0.51	0.09	63,63,63,63	0
57	MG	2A	3353	1/1	0.52	0.32	69,69,69,69	0
57	MG	2a	3031	1/1	0.52	0.47	64,64,64,64	0
57	MG	1A	3402	1/1	0.52	0.20	66,66,66,66	0
57	MG	1A	4117	1/1	0.55	0.10	59,59,59,59	0
57	MG	2A	3356	1/1	0.56	0.21	68,68,68,68	0
57	MG	1A	3899	1/1	0.56	0.24	38,38,38,38	0
57	MG	1a	3245	1/1	0.57	0.26	66,66,66,66	0
57	MG	2A	3215	1/1	0.57	0.23	64,64,64,64	0
57	MG	2A	3083	1/1	0.57	0.24	62,62,62,62	0
57	MG	2A	3867	1/1	0.57	0.15	47,47,47,47	0
57	MG	2a	3186	1/1	0.58	0.46	70,70,70,70	0
57	MG	1A	3483	1/1	0.58	0.20	74,74,74,74	0
57	MG	2a	3058	1/1	0.58	0.24	61,61,61,61	0
57	MG	2a	3235	1/1	0.58	0.12	73,73,73,73	0
57	MG	1a	3201	1/1	0.58	0.09	59,59,59,59	0
57	MG	1A	3431	1/1	0.58	0.16	44,44,44,44	0
57	MG	2A	3724	1/1	0.59	0.15	69,69,69,69	0
57	MG	1A	3818	1/1	0.59	0.18	57,57,57,57	0
57	MG	2A	3923	1/1	0.60	0.10	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3862	1/1	0.60	0.10	45,45,45,45	0
57	MG	2A	3257	1/1	0.60	0.20	62,62,62,62	0
57	MG	2a	3153	1/1	0.61	0.14	75,75,75,75	0
57	MG	1A	3570	1/1	0.61	0.21	52,52,52,52	0
59	ZN	14	501	1/1	0.61	0.09	106,106,106,106	0
57	MG	2a	3154	1/1	0.62	0.16	71,71,71,71	0
57	MG	2A	3176	1/1	0.63	0.14	64,64,64,64	0
57	MG	1A	3521	1/1	0.63	0.20	57,57,57,57	0
57	MG	2a	3261	1/1	0.63	0.23	68,68,68,68	0
57	MG	1A	3349	1/1	0.64	0.16	46,46,46,46	0
57	MG	2a	3042	1/1	0.64	0.28	61,61,61,61	0
57	MG	2a	3199	1/1	0.64	0.14	67,67,67,67	0
57	MG	2A	3921	1/1	0.64	0.27	60,60,60,60	0
57	MG	1A	4208	1/1	0.64	0.35	53,53,53,53	0
57	MG	1A	3052	1/1	0.64	0.22	53,53,53,53	0
57	MG	1A	3492	1/1	0.64	0.24	64,64,64,64	0
57	MG	2A	3599	1/1	0.64	0.14	54,54,54,54	0
57	MG	2a	3002	1/1	0.64	0.56	69,69,69,69	0
57	MG	2A	3478	1/1	0.64	0.23	36,36,36,36	0
57	MG	2A	3341	1/1	0.65	0.98	66,66,66,66	0
57	MG	1A	3805	1/1	0.65	0.17	35,35,35,35	0
57	MG	1A	4098	1/1	0.65	0.12	41,41,41,41	0
57	MG	2A	3093	1/1	0.65	0.11	68,68,68,68	0
57	MG	1a	3217	1/1	0.66	0.13	56,56,56,56	0
57	MG	1a	3230	1/1	0.66	0.21	65,65,65,65	0
57	MG	1A	4274	1/1	0.66	0.46	69,69,69,69	0
57	MG	2A	3850	1/1	0.66	0.09	59,59,59,59	0
57	MG	2A	3875	1/1	0.66	0.20	65,65,65,65	0
57	MG	1A	3439	1/1	0.66	0.24	66,66,66,66	0
57	MG	1A	4090	1/1	0.66	0.10	50,50,50,50	0
57	MG	1A	3500	1/1	0.66	0.26	54,54,54,54	0
57	MG	2A	3396	1/1	0.66	0.13	75,75,75,75	0
57	MG	1a	3015	1/1	0.66	0.14	47,47,47,47	0
57	MG	1A	3480	1/1	0.67	0.36	53,53,53,53	0
57	MG	1A	3099	1/1	0.67	0.11	56,56,56,56	0
57	MG	1A	4065	1/1	0.67	0.10	42,42,42,42	0
57	MG	2A	3573	1/1	0.67	0.13	64,64,64,64	0
57	MG	2A	3220	1/1	0.67	0.24	66,66,66,66	0
57	MG	1a	3022	1/1	0.68	0.31	58,58,58,58	0
57	MG	1A	4167	1/1	0.68	0.14	65,65,65,65	0
57	MG	1A	3137	1/1	0.68	0.18	61,61,61,61	0
57	MG	2A	3001	1/1	0.68	0.27	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	2a	3090	1/1	0.68	0.12	59,59,59,59	0
57	MG	1a	3141	1/1	0.69	0.20	64,64,64,64	0
57	MG	2a	3151	1/1	0.69	0.21	65,65,65,65	0
57	MG	1A	4200	1/1	0.69	0.07	49,49,49,49	0
57	MG	2A	3397	1/1	0.69	0.19	41,41,41,41	0
57	MG	2a	3253	1/1	0.69	0.12	59,59,59,59	0
57	MG	1a	3158	1/1	0.69	0.12	48,48,48,48	0
57	MG	2A	3107	1/1	0.69	0.21	63,63,63,63	0
57	MG	1A	4183	1/1	0.69	0.18	49,49,49,49	0
57	MG	1a	3166	1/1	0.70	0.16	79,79,79,79	0
57	MG	2A	3016	1/1	0.70	0.14	62,62,62,62	0
57	MG	2A	3567	1/1	0.70	0.10	57,57,57,57	0
57	MG	2a	3192	1/1	0.70	0.32	75,75,75,75	0
57	MG	2A	3608	1/1	0.70	0.17	44,44,44,44	0
57	MG	2a	3038	1/1	0.70	0.13	67,67,67,67	0
57	MG	2a	3050	1/1	0.70	0.67	69,69,69,69	0
57	MG	2A	3840	1/1	0.71	0.71	57,57,57,57	0
57	MG	1A	3515	1/1	0.71	0.23	53,53,53,53	0
57	MG	1a	3084	1/1	0.71	0.13	64,64,64,64	0
57	MG	2a	3093	1/1	0.71	0.13	53,53,53,53	0
57	MG	1A	4163	1/1	0.71	0.16	58,58,58,58	0
57	MG	1A	3061	1/1	0.71	0.16	40,40,40,40	0
57	MG	2A	3629	1/1	0.72	0.17	49,49,49,49	0
57	MG	1A	4079	1/1	0.72	0.18	43,43,43,43	0
57	MG	1A	3314	1/1	0.72	0.17	57,57,57,57	0
57	MG	2A	3812	1/1	0.72	0.15	49,49,49,49	0
57	MG	1A	3563	1/1	0.72	0.28	53,53,53,53	0
57	MG	2a	3163	1/1	0.72	0.24	67,67,67,67	0
57	MG	1a	3027	1/1	0.72	0.19	65,65,65,65	0
57	MG	1A	4136	1/1	0.72	0.13	42,42,42,42	0
57	MG	2a	3140	1/1	0.72	0.31	58,58,58,58	0
57	MG	2a	3126	1/1	0.73	0.14	66,66,66,66	0
57	MG	2A	3590	1/1	0.73	0.19	55,55,55,55	0
57	MG	1a	3095	1/1	0.73	0.27	57,57,57,57	0
57	MG	1a	3215	1/1	0.73	0.12	54,54,54,54	0
57	MG	2A	3615	1/1	0.73	0.17	58,58,58,58	0
57	MG	2a	3268	1/1	0.73	0.16	74,74,74,74	0
57	MG	2A	3611	1/1	0.73	0.16	41,41,41,41	0
57	MG	2a	3010	1/1	0.73	0.13	64,64,64,64	0
57	MG	2A	3261	1/1	0.73	0.27	64,64,64,64	0
57	MG	1a	3106	1/1	0.73	0.19	45,45,45,45	0
57	MG	1a	3083	1/1	0.74	0.18	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	3196	1/1	0.74	0.16	58,58,58,58	0
57	MG	2A	3116	1/1	0.74	0.17	65,65,65,65	0
57	MG	2A	3427	1/1	0.74	0.18	54,54,54,54	0
57	MG	2A	3322	1/1	0.74	0.29	50,50,50,50	0
57	MG	2A	3644	1/1	0.74	0.18	37,37,37,37	0
57	MG	2A	3918	1/1	0.74	0.13	56,56,56,56	0
57	MG	1A	3502	1/1	0.74	0.34	64,64,64,64	0
57	MG	2A	3026	1/1	0.74	0.28	46,46,46,46	0
57	MG	2A	3492	1/1	0.74	0.20	54,54,54,54	0
57	MG	2A	3638	1/1	0.74	0.16	34,34,34,34	0
57	MG	1A	4251	1/1	0.74	0.09	49,49,49,49	0
57	MG	1A	3600	1/1	0.74	0.15	54,54,54,54	0
57	MG	1A	4180	1/1	0.74	0.12	31,31,31,31	0
57	MG	2A	3070	1/1	0.74	0.19	63,63,63,63	0
57	MG	1a	3173	1/1	0.74	0.12	44,44,44,44	0
57	MG	2a	3174	1/1	0.74	0.13	66,66,66,66	0
57	MG	1a	3138	1/1	0.74	0.15	69,69,69,69	0
57	MG	1A	3941	1/1	0.75	0.11	51,51,51,51	0
57	MG	2A	3511	1/1	0.75	0.25	48,48,48,48	0
57	MG	2a	3120	1/1	0.75	0.15	52,52,52,52	0
57	MG	1a	3248	1/1	0.75	0.19	73,73,73,73	0
57	MG	2A	3256	1/1	0.75	0.17	61,61,61,61	0
57	MG	1A	3977	1/1	0.75	0.37	50,50,50,50	0
57	MG	2A	3410	1/1	0.75	0.25	70,70,70,70	0
57	MG	1A	3957	1/1	0.75	0.15	54,54,54,54	0
57	MG	2a	3101	1/1	0.75	0.19	57,57,57,57	0
57	MG	1A	3419	1/1	0.75	0.15	42,42,42,42	0
57	MG	1a	3183	1/1	0.75	0.10	58,58,58,58	0
57	MG	1A	3094	1/1	0.75	0.15	33,33,33,33	0
57	MG	1A	4210	1/1	0.75	0.19	53,53,53,53	0
57	MG	2A	3584	1/1	0.75	0.14	34,34,34,34	0
57	MG	2A	3164	1/1	0.75	0.17	56,56,56,56	0
57	MG	1A	3546	1/1	0.75	0.18	59,59,59,59	0
57	MG	2A	3263	1/1	0.76	0.29	49,49,49,49	0
57	MG	2A	3328	1/1	0.76	0.18	46,46,46,46	0
57	MG	1A	4068	1/1	0.76	0.12	26,26,26,26	0
57	MG	1a	3237	1/1	0.76	0.38	77,77,77,77	0
57	MG	1a	3040	1/1	0.76	0.29	58,58,58,58	0
57	MG	2A	3482	1/1	0.76	0.62	53,53,53,53	0
57	MG	2A	3354	1/1	0.76	0.21	66,66,66,66	0
57	MG	2A	3660	1/1	0.76	0.18	56,56,56,56	0
57	MG	1A	3792	1/1	0.76	0.20	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	2A	3515	1/1	0.76	0.13	63,63,63,63	0
57	MG	2A	3368	1/1	0.76	0.31	47,47,47,47	0
57	MG	2a	3009	1/1	0.76	0.16	62,62,62,62	0
57	MG	2A	3065	1/1	0.76	0.17	48,48,48,48	0
57	MG	1A	3873	1/1	0.76	0.14	46,46,46,46	0
57	MG	2A	3648	1/1	0.76	0.12	59,59,59,59	0
57	MG	2A	3885	1/1	0.76	0.07	54,54,54,54	0
57	MG	2A	3272	1/1	0.76	0.14	57,57,57,57	0
57	MG	1A	3940	1/1	0.76	0.10	38,38,38,38	0
57	MG	2A	3315	1/1	0.76	0.36	61,61,61,61	0
57	MG	2a	3027	1/1	0.76	0.98	74,74,74,74	0
57	MG	2A	3496	1/1	0.76	0.34	71,71,71,71	0
57	MG	2A	3941	1/1	0.76	0.14	66,66,66,66	0
57	MG	2A	3087	1/1	0.76	0.17	47,47,47,47	0
57	MG	2A	3146	1/1	0.77	0.27	38,38,38,38	0
57	MG	1a	3075	1/1	0.77	0.21	53,53,53,53	0
57	MG	1A	3411	1/1	0.77	0.20	55,55,55,55	0
57	MG	1A	4197	1/1	0.77	0.33	65,65,65,65	0
57	MG	2A	3486	1/1	0.77	0.28	61,61,61,61	0
57	MG	2A	3190	1/1	0.77	0.12	68,68,68,68	0
57	MG	2a	3238	1/1	0.77	0.17	48,48,48,48	0
57	MG	2A	3880	1/1	0.77	0.15	35,35,35,35	0
57	MG	1A	3781	1/1	0.77	0.16	68,68,68,68	0
57	MG	2A	3791	1/1	0.77	0.12	60,60,60,60	0
57	MG	2A	3407	1/1	0.77	0.37	55,55,55,55	0
57	MG	2A	3242	1/1	0.77	0.31	64,64,64,64	0
57	MG	1A	3440	1/1	0.77	0.24	46,46,46,46	0
57	MG	2a	3055	1/1	0.77	0.16	57,57,57,57	0
57	MG	1A	4051	1/1	0.77	0.13	44,44,44,44	0
57	MG	2a	3149	1/1	0.77	0.11	77,77,77,77	0
57	MG	1A	3284	1/1	0.77	0.25	58,58,58,58	0
57	MG	1A	3922	1/1	0.77	0.19	44,44,44,44	0
57	MG	2a	3020	1/1	0.77	0.24	65,65,65,65	0
57	MG	1A	4292	1/1	0.77	0.28	57,57,57,57	0
57	MG	1A	3860	1/1	0.77	0.21	38,38,38,38	0
57	MG	2A	3259	1/1	0.77	0.15	71,71,71,71	0
57	MG	1A	3121	1/1	0.78	0.33	41,41,41,41	0
57	MG	1a	3195	1/1	0.78	0.12	45,45,45,45	0
57	MG	1A	3550	1/1	0.78	0.21	33,33,33,33	0
57	MG	2A	3865	1/1	0.78	0.12	50,50,50,50	0
57	MG	1a	3247	1/1	0.78	0.18	73,73,73,73	0
57	MG	2A	3893	1/1	0.78	0.09	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	3403	1/1	0.78	0.19	50,50,50,50	0
57	MG	1A	4077	1/1	0.78	0.13	33,33,33,33	0
57	MG	2A	3747	1/1	0.78	0.26	58,58,58,58	0
57	MG	1A	3503	1/1	0.78	0.16	43,43,43,43	0
57	MG	2A	3953	1/1	0.78	0.44	69,69,69,69	0
57	MG	2a	3054	1/1	0.78	0.14	72,72,72,72	0
57	MG	1A	3113	1/1	0.78	0.20	26,26,26,26	0
57	MG	1a	3097	1/1	0.78	0.19	52,52,52,52	0
57	MG	2a	3007	1/1	0.78	0.21	51,51,51,51	0
57	MG	2A	3329	1/1	0.78	0.34	57,57,57,57	0
57	MG	1A	3843	1/1	0.78	0.15	45,45,45,45	0
57	MG	2A	3575	1/1	0.78	0.21	64,64,64,64	0
57	MG	1A	4097	1/1	0.78	0.13	51,51,51,51	0
57	MG	2a	3030	1/1	0.78	0.56	66,66,66,66	0
57	MG	1A	3924	1/1	0.78	0.12	41,41,41,41	0
57	MG	2a	3168	1/1	0.78	0.15	60,60,60,60	0
57	MG	1A	3268	1/1	0.78	0.14	55,55,55,55	0
57	MG	2A	3758	1/1	0.78	0.10	60,60,60,60	0
57	MG	1A	4239	1/1	0.78	0.15	64,64,64,64	0
57	MG	2A	3905	1/1	0.78	0.18	32,32,32,32	0
57	MG	2A	3325	1/1	0.78	0.13	54,54,54,54	0
57	MG	1A	3915	1/1	0.78	0.09	30,30,30,30	0
57	MG	2A	3299	1/1	0.79	0.12	65,65,65,65	0
57	MG	1A	3985	1/1	0.79	0.05	61,61,61,61	0
57	MG	2a	3190	1/1	0.79	0.12	47,47,47,47	0
57	MG	1A	4120	1/1	0.79	0.21	53,53,53,53	0
57	MG	1A	4003	1/1	0.79	0.13	39,39,39,39	0
57	MG	2a	3264	1/1	0.79	0.15	64,64,64,64	0
57	MG	1A	4128	1/1	0.79	0.09	53,53,53,53	0
57	MG	1a	3069	1/1	0.79	0.20	53,53,53,53	0
57	MG	2a	3248	1/1	0.79	0.11	59,59,59,59	0
57	MG	1a	3199	1/1	0.79	0.10	68,68,68,68	0
57	MG	1A	3883	1/1	0.79	0.19	24,24,24,24	0
57	MG	2a	3107	1/1	0.79	0.17	59,59,59,59	0
57	MG	1A	4033	1/1	0.79	0.21	23,23,23,23	0
57	MG	2A	3906	1/1	0.79	0.16	33,33,33,33	0
57	MG	2A	3279	1/1	0.79	0.21	67,67,67,67	0
57	MG	2A	3711	1/1	0.79	0.22	36,36,36,36	0
57	MG	2a	3222	1/1	0.79	0.17	51,51,51,51	0
57	MG	2A	3273	1/1	0.79	0.27	69,69,69,69	0
57	MG	2A	3154	1/1	0.79	0.13	54,54,54,54	0
57	MG	1A	4075	1/1	0.79	0.06	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	3604	1/1	0.79	0.15	54,54,54,54	0
57	MG	2a	3091	1/1	0.79	0.10	69,69,69,69	0
57	MG	2A	3369	1/1	0.80	0.22	58,58,58,58	0
57	MG	1a	3209	1/1	0.80	0.12	44,44,44,44	0
57	MG	1a	3028	1/1	0.80	0.18	57,57,57,57	0
57	MG	1a	3176	1/1	0.80	0.21	59,59,59,59	0
57	MG	1A	3980	1/1	0.80	0.12	31,31,31,31	0
57	MG	1a	3178	1/1	0.80	0.13	43,43,43,43	0
57	MG	1A	3505	1/1	0.80	0.17	66,66,66,66	0
57	MG	1a	3003	1/1	0.80	0.11	61,61,61,61	0
57	MG	2A	3730	1/1	0.80	0.14	55,55,55,55	0
57	MG	2A	3208	1/1	0.80	0.18	49,49,49,49	0
57	MG	2a	3165	1/1	0.80	0.14	69,69,69,69	0
57	MG	2a	3203	1/1	0.80	0.11	62,62,62,62	0
57	MG	2A	3229	1/1	0.80	0.24	47,47,47,47	0
57	MG	2A	3914	1/1	0.80	0.10	51,51,51,51	0
57	MG	1A	3467	1/1	0.80	0.28	53,53,53,53	0
57	MG	1A	4174	1/1	0.80	0.09	57,57,57,57	0
57	MG	2A	3792	1/1	0.80	0.12	37,37,37,37	0
57	MG	2a	3234	1/1	0.80	0.08	59,59,59,59	0
57	MG	1A	3737	1/1	0.80	0.15	54,54,54,54	0
57	MG	1A	4063	1/1	0.80	0.04	54,54,54,54	0
57	MG	1A	3313	1/1	0.80	0.14	42,42,42,42	0
57	MG	1a	3220	1/1	0.80	0.07	63,63,63,63	0
57	MG	1A	3447	1/1	0.80	0.15	60,60,60,60	0
57	MG	1A	4108	1/1	0.80	0.20	50,50,50,50	0
57	MG	1a	3059	1/1	0.80	0.22	64,64,64,64	0
57	MG	1A	3271	1/1	0.80	0.37	49,49,49,49	0
57	MG	1A	3895	1/1	0.80	0.13	49,49,49,49	0
57	MG	2A	3285	1/1	0.80	0.14	52,52,52,52	0
57	MG	1A	4082	1/1	0.80	0.32	55,55,55,55	0
57	MG	2A	3447	1/1	0.80	0.38	49,49,49,49	0
57	MG	2A	3554	1/1	0.80	0.19	65,65,65,65	0
57	MG	1a	3148	1/1	0.80	0.17	59,59,59,59	0
57	MG	1A	3282	1/1	0.80	0.15	53,53,53,53	0
57	MG	2A	3509	1/1	0.80	0.18	62,62,62,62	0
57	MG	2a	3076	1/1	0.81	0.10	53,53,53,53	0
57	MG	1A	3557	1/1	0.81	0.19	62,62,62,62	0
57	MG	2A	3049	1/1	0.81	0.24	52,52,52,52	0
57	MG	1a	3152	1/1	0.81	0.16	47,47,47,47	0
57	MG	2a	3005	1/1	0.81	0.10	70,70,70,70	0
57	MG	2A	3275	1/1	0.81	0.14	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	3037	1/1	0.81	0.70	75,75,75,75	0
57	MG	2A	3931	1/1	0.81	0.12	44,44,44,44	0
57	MG	1a	3100	1/1	0.81	0.17	53,53,53,53	0
57	MG	2a	3211	1/1	0.81	0.08	58,58,58,58	0
57	MG	2A	3943	1/1	0.81	0.23	57,57,57,57	0
57	MG	2A	3283	1/1	0.81	0.15	50,50,50,50	0
57	MG	2a	3049	1/1	0.81	0.10	53,53,53,53	0
57	MG	2A	3797	1/1	0.81	0.15	58,58,58,58	0
57	MG	2A	3068	1/1	0.81	0.23	50,50,50,50	0
57	MG	1a	3067	1/1	0.81	0.20	55,55,55,55	0
57	MG	1A	3520	1/1	0.81	0.23	47,47,47,47	0
57	MG	2a	3043	1/1	0.81	0.13	61,61,61,61	0
57	MG	2a	3011	1/1	0.81	0.22	64,64,64,64	0
57	MG	1a	3190	1/1	0.81	0.10	54,54,54,54	0
57	MG	1A	3444	1/1	0.81	0.21	56,56,56,56	0
57	MG	2A	3209	1/1	0.81	0.14	54,54,54,54	0
57	MG	1a	3029	1/1	0.81	0.18	47,47,47,47	0
57	MG	2A	3523	1/1	0.81	0.28	46,46,46,46	0
57	MG	1A	3999	1/1	0.81	0.12	49,49,49,49	0
57	MG	1a	3113	1/1	0.81	0.21	52,52,52,52	0
57	MG	2A	3678	1/1	0.81	0.14	58,58,58,58	0
57	MG	2A	3244	1/1	0.81	0.11	66,66,66,66	0
57	MG	1A	3316	1/1	0.81	0.18	47,47,47,47	0
57	MG	1A	4159	1/1	0.81	0.12	41,41,41,41	0
57	MG	2A	3199	1/1	0.81	0.10	63,63,63,63	0
57	MG	2A	3776	1/1	0.81	0.18	62,62,62,62	0
57	MG	2A	3426	1/1	0.81	0.17	57,57,57,57	0
57	MG	2A	3741	1/1	0.81	0.22	54,54,54,54	0
57	MG	1A	3949	1/1	0.81	0.17	53,53,53,53	0
57	MG	1A	3739	1/1	0.81	0.15	42,42,42,42	0
57	MG	2A	3336	1/1	0.81	0.23	55,55,55,55	0
57	MG	2A	3833	1/1	0.81	0.22	62,62,62,62	0
57	MG	1A	3849	1/1	0.81	0.15	48,48,48,48	0
57	MG	2A	3675	1/1	0.81	0.17	45,45,45,45	0
57	MG	2A	3343	1/1	0.82	0.18	51,51,51,51	0
57	MG	1A	4122	1/1	0.82	0.12	50,50,50,50	0
57	MG	1A	3127	1/1	0.82	0.23	38,38,38,38	0
57	MG	1A	4151	1/1	0.82	0.18	50,50,50,50	0
57	MG	2a	3127	1/1	0.82	0.11	59,59,59,59	0
57	MG	1A	3459	1/1	0.82	0.16	45,45,45,45	0
57	MG	1a	3061	1/1	0.82	0.17	46,46,46,46	0
57	MG	1A	4279	1/1	0.82	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	3890	1/1	0.82	0.20	39,39,39,39	0
57	MG	1A	4271	1/1	0.82	0.11	48,48,48,48	0
57	MG	2A	3658	1/1	0.82	0.13	52,52,52,52	0
57	MG	2A	3331	1/1	0.82	0.11	58,58,58,58	0
57	MG	2A	3715	1/1	0.82	0.20	43,43,43,43	0
57	MG	1a	3056	1/1	0.82	0.16	49,49,49,49	0
57	MG	2A	3606	1/1	0.82	0.10	54,54,54,54	0
57	MG	2A	3924	1/1	0.82	0.08	71,71,71,71	0
57	MG	2A	3857	1/1	0.82	0.15	59,59,59,59	0
57	MG	1A	4255	1/1	0.82	0.11	53,53,53,53	0
57	MG	1a	3193	1/1	0.82	0.13	57,57,57,57	0
57	MG	1A	3599	1/1	0.82	0.20	71,71,71,71	0
57	MG	2A	3888	1/1	0.82	0.14	37,37,37,37	0
57	MG	2a	3158	1/1	0.82	0.18	66,66,66,66	0
57	MG	2a	3048	1/1	0.82	0.11	53,53,53,53	0
57	MG	2A	3826	1/1	0.82	0.25	49,49,49,49	0
57	MG	1A	3478	1/1	0.82	0.17	46,46,46,46	0
57	MG	1A	3862	1/1	0.82	0.20	56,56,56,56	0
57	MG	1a	3001	1/1	0.82	0.09	51,51,51,51	0
57	MG	1a	3140	1/1	0.82	0.35	51,51,51,51	0
57	MG	2A	3128	1/1	0.82	0.14	48,48,48,48	0
57	MG	2A	3082	1/1	0.82	0.18	52,52,52,52	0
57	MG	2a	3236	1/1	0.82	0.19	63,63,63,63	0
57	MG	1a	3042	1/1	0.82	0.29	57,57,57,57	0
57	MG	2a	3133	1/1	0.82	0.49	60,60,60,60	0
57	MG	2A	3761	1/1	0.82	0.19	37,37,37,37	0
57	MG	1a	3157	1/1	0.82	0.16	51,51,51,51	0
57	MG	1A	3808	1/1	0.82	0.21	22,22,22,22	0
57	MG	1A	3537	1/1	0.82	0.12	60,60,60,60	0
57	MG	2A	3780	1/1	0.82	0.15	47,47,47,47	0
57	MG	1a	3214	1/1	0.82	0.06	57,57,57,57	0
57	MG	1a	3109	1/1	0.82	0.22	55,55,55,55	0
57	MG	2A	3163	1/1	0.82	0.15	54,54,54,54	0
57	MG	1A	3910	1/1	0.82	0.14	15,15,15,15	0
57	MG	1A	3399	1/1	0.82	0.26	51,51,51,51	0
57	MG	2A	3149	1/1	0.82	0.17	66,66,66,66	0
57	MG	2A	3738	1/1	0.83	0.11	56,56,56,56	0
57	MG	2a	3209	1/1	0.83	0.06	63,63,63,63	0
57	MG	2A	3033	1/1	0.83	0.20	54,54,54,54	0
57	MG	1A	3436	1/1	0.83	0.25	36,36,36,36	0
57	MG	1A	3337	1/1	0.83	0.34	52,52,52,52	0
57	MG	2A	3338	1/1	0.83	0.14	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	2A	3213	1/1	0.83	0.24	55,55,55,55	0
57	MG	2A	3355	1/1	0.83	0.20	69,69,69,69	0
57	MG	1a	3191	1/1	0.83	0.15	56,56,56,56	0
57	MG	2A	3585	1/1	0.83	0.16	63,63,63,63	0
57	MG	2A	3773	1/1	0.83	0.07	46,46,46,46	0
57	MG	2A	3103	1/1	0.83	0.25	49,49,49,49	0
57	MG	2A	3948	1/1	0.83	0.34	69,69,69,69	0
57	MG	1A	3405	1/1	0.83	0.25	30,30,30,30	0
57	MG	2A	3174	1/1	0.83	0.37	61,61,61,61	0
57	MG	1A	4296	1/1	0.83	0.10	61,61,61,61	0
57	MG	2A	3253	1/1	0.83	0.17	66,66,66,66	0
57	MG	2A	3684	1/1	0.83	0.11	43,43,43,43	0
57	MG	1A	3508	1/1	0.83	0.19	37,37,37,37	0
57	MG	1A	3771	1/1	0.83	0.15	23,23,23,23	0
57	MG	2A	3411	1/1	0.83	0.39	51,51,51,51	0
57	MG	2A	3742	1/1	0.83	0.12	52,52,52,52	0
57	MG	2A	3860	1/1	0.83	0.14	57,57,57,57	0
57	MG	1A	3733	1/1	0.83	0.29	52,52,52,52	0
57	MG	1A	3197	1/1	0.83	0.12	54,54,54,54	0
57	MG	2A	3056	1/1	0.83	0.16	53,53,53,53	0
57	MG	1A	3250	1/1	0.83	0.44	34,34,34,34	0
57	MG	2a	3250	1/1	0.83	0.14	49,49,49,49	0
57	MG	2a	3036	1/1	0.83	0.12	61,61,61,61	0
57	MG	2A	3866	1/1	0.83	0.17	54,54,54,54	0
57	MG	1A	3395	1/1	0.83	0.22	45,45,45,45	0
57	MG	2A	3640	1/1	0.83	0.13	60,60,60,60	0
57	MG	1A	3182	1/1	0.83	0.22	33,33,33,33	0
57	MG	1a	3151	1/1	0.83	0.27	71,71,71,71	0
57	MG	1A	4278	1/1	0.83	0.21	30,30,30,30	0
57	MG	1A	3543	1/1	0.83	0.14	48,48,48,48	0
57	MG	2a	3164	1/1	0.83	0.09	69,69,69,69	0
57	MG	1a	3224	1/1	0.83	0.09	52,52,52,52	0
57	MG	1A	3315	1/1	0.83	0.19	45,45,45,45	0
57	MG	1a	3180	1/1	0.83	0.16	38,38,38,38	0
57	MG	2A	3317	1/1	0.83	0.11	70,70,70,70	0
57	MG	1a	3197	1/1	0.83	0.19	64,64,64,64	0
57	MG	2A	3412	1/1	0.83	0.35	55,55,55,55	0
57	MG	1a	3165	1/1	0.83	0.10	47,47,47,47	0
57	MG	1A	4140	1/1	0.83	0.10	43,43,43,43	0
57	MG	1a	3125	1/1	0.83	0.18	54,54,54,54	0
57	MG	1a	3202	1/1	0.83	0.08	55,55,55,55	0
57	MG	2A	3483	1/1	0.84	0.16	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3908	1/1	0.84	0.07	57,57,57,57	0
57	MG	2A	3692	1/1	0.84	0.14	33,33,33,33	0
57	MG	1a	3171	1/1	0.84	0.17	42,42,42,42	0
57	MG	1A	3386	1/1	0.84	0.13	45,45,45,45	0
57	MG	1a	3244	1/1	0.84	0.14	65,65,65,65	0
57	MG	2A	3625	1/1	0.84	0.14	44,44,44,44	0
57	MG	1a	3207	1/1	0.84	0.17	62,62,62,62	0
57	MG	1A	4119	1/1	0.84	0.10	58,58,58,58	0
57	MG	1A	3223	1/1	0.84	0.18	46,46,46,46	0
57	MG	2a	3122	1/1	0.84	0.19	67,67,67,67	0
57	MG	2a	3014	1/1	0.84	0.20	58,58,58,58	0
57	MG	1A	3083	1/1	0.84	0.23	58,58,58,58	0
57	MG	2a	3118	1/1	0.84	0.19	53,53,53,53	0
57	MG	1a	3211	1/1	0.84	0.10	54,54,54,54	0
57	MG	1a	3168	1/1	0.84	0.10	35,35,35,35	0
57	MG	1a	3136	1/1	0.84	0.14	52,52,52,52	0
57	MG	1a	3187	1/1	0.84	0.11	57,57,57,57	0
57	MG	2A	3557	1/1	0.84	0.11	60,60,60,60	0
57	MG	1A	4006	1/1	0.84	0.17	47,47,47,47	0
57	MG	2A	3456	1/1	0.84	0.14	64,64,64,64	0
57	MG	1A	3626	1/1	0.84	0.42	44,44,44,44	0
57	MG	1A	3506	1/1	0.84	0.24	44,44,44,44	0
57	MG	1A	3518	1/1	0.84	0.14	43,43,43,43	0
57	MG	1A	3104	1/1	0.84	0.25	53,53,53,53	0
57	MG	2A	3762	1/1	0.84	0.11	57,57,57,57	0
57	MG	2a	3225	1/1	0.84	0.15	45,45,45,45	0
57	MG	2A	3359	1/1	0.84	0.11	56,56,56,56	0
57	MG	1A	3228	1/1	0.84	0.13	36,36,36,36	0
57	MG	1A	3261	1/1	0.84	0.20	45,45,45,45	0
57	MG	1A	3931	1/1	0.84	0.14	73,73,73,73	0
57	MG	2A	3804	1/1	0.84	0.15	60,60,60,60	0
57	MG	2A	3466	1/1	0.84	0.17	40,40,40,40	0
57	MG	2a	3129	1/1	0.84	0.14	61,61,61,61	0
57	MG	2A	3381	1/1	0.84	0.21	62,62,62,62	0
57	MG	2A	3899	1/1	0.84	0.10	51,51,51,51	0
57	MG	2A	3951	1/1	0.84	0.10	42,42,42,42	0
57	MG	2a	3110	1/1	0.84	0.42	56,56,56,56	0
57	MG	2A	3377	1/1	0.84	0.21	59,59,59,59	0
57	MG	2A	3111	1/1	0.84	0.24	47,47,47,47	0
57	MG	2A	3312	1/1	0.84	0.28	56,56,56,56	0
57	MG	2A	3731	1/1	0.84	0.17	67,67,67,67	0
57	MG	2A	3061	1/1	0.84	0.26	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	3008	1/1	0.84	0.18	53,53,53,53	0
57	MG	1A	3363	1/1	0.84	0.29	48,48,48,48	0
57	MG	2a	3097	1/1	0.84	0.26	56,56,56,56	0
57	MG	1A	3401	1/1	0.84	0.12	45,45,45,45	0
57	MG	1A	4166	1/1	0.84	0.19	48,48,48,48	0
57	MG	2a	3041	1/1	0.84	0.25	50,50,50,50	0
57	MG	1A	4147	1/1	0.84	0.14	29,29,29,29	0
57	MG	1a	3175	1/1	0.84	0.08	57,57,57,57	0
57	MG	2A	3641	1/1	0.84	0.13	38,38,38,38	0
57	MG	1A	4009	1/1	0.84	0.20	43,43,43,43	0
57	MG	2A	3045	1/1	0.84	0.13	59,59,59,59	0
57	MG	1A	3761	1/1	0.84	0.17	27,27,27,27	0
57	MG	1A	3857	1/1	0.84	0.13	45,45,45,45	0
57	MG	2A	3697	1/1	0.84	0.17	30,30,30,30	0
57	MG	1A	3556	1/1	0.84	0.11	56,56,56,56	0
57	MG	2A	3298	1/1	0.84	0.30	57,57,57,57	0
57	MG	2A	3712	1/1	0.84	0.12	49,49,49,49	0
57	MG	1a	3198	1/1	0.84	0.13	47,47,47,47	0
57	MG	1A	4226	1/1	0.85	0.21	28,28,28,28	0
57	MG	2A	3465	1/1	0.85	0.18	53,53,53,53	0
57	MG	2A	3627	1/1	0.85	0.10	44,44,44,44	0
57	MG	2a	3135	1/1	0.85	0.12	65,65,65,65	0
57	MG	2A	3088	1/1	0.85	0.13	48,48,48,48	0
57	MG	2A	3835	1/1	0.85	0.11	41,41,41,41	0
57	MG	2A	3170	1/1	0.85	0.27	56,56,56,56	0
57	MG	1A	3486	1/1	0.85	0.15	51,51,51,51	0
57	MG	1A	4093	1/1	0.85	0.20	44,44,44,44	0
57	MG	2a	3035	1/1	0.85	0.11	54,54,54,54	0
57	MG	2A	3043	1/1	0.85	0.19	42,42,42,42	0
57	MG	2A	3710	1/1	0.85	0.20	33,33,33,33	0
57	MG	1a	3063	1/1	0.85	0.13	45,45,45,45	0
57	MG	2A	3438	1/1	0.85	0.25	51,51,51,51	0
57	MG	2A	3305	1/1	0.85	0.14	60,60,60,60	0
57	MG	1A	3728	1/1	0.85	0.22	46,46,46,46	0
57	MG	1A	3312	1/1	0.85	0.17	42,42,42,42	0
57	MG	1A	3355	1/1	0.85	0.29	64,64,64,64	0
57	MG	2a	3147	1/1	0.85	0.09	50,50,50,50	0
57	MG	2A	3367	1/1	0.85	0.12	58,58,58,58	0
57	MG	2A	3787	1/1	0.85	0.20	59,59,59,59	0
57	MG	1A	3528	1/1	0.85	0.13	53,53,53,53	0
57	MG	1a	3007	1/1	0.85	0.29	49,49,49,49	0
57	MG	2A	3337	1/1	0.85	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	3318	1/1	0.85	0.19	69,69,69,69	0
57	MG	2A	3120	1/1	0.85	0.11	50,50,50,50	0
57	MG	2A	3109	1/1	0.85	0.20	61,61,61,61	0
57	MG	1A	3382	1/1	0.85	0.15	62,62,62,62	0
57	MG	2A	3278	1/1	0.85	0.15	60,60,60,60	0
57	MG	2a	3044	1/1	0.85	0.14	50,50,50,50	0
57	MG	2A	3291	1/1	0.85	0.37	59,59,59,59	0
57	MG	1A	3362	1/1	0.85	0.11	43,43,43,43	0
57	MG	1A	3845	1/1	0.85	0.14	25,25,25,25	0
57	MG	1a	3002	1/1	0.85	0.16	50,50,50,50	0
57	MG	1A	3186	1/1	0.85	0.17	32,32,32,32	0
57	MG	2A	3493	1/1	0.85	0.20	61,61,61,61	0
57	MG	1A	3624	1/1	0.85	0.22	58,58,58,58	0
57	MG	2A	3193	1/1	0.85	0.18	45,45,45,45	0
57	MG	2a	3028	1/1	0.85	0.17	55,55,55,55	0
57	MG	1A	3226	1/1	0.85	0.12	36,36,36,36	0
57	MG	2a	3094	1/1	0.85	0.14	57,57,57,57	0
57	MG	1A	3708	1/1	0.85	0.28	42,42,42,42	0
57	MG	2A	3400	1/1	0.85	0.19	58,58,58,58	0
57	MG	1A	3631	1/1	0.85	0.20	39,39,39,39	0
57	MG	1a	3049	1/1	0.85	0.34	51,51,51,51	0
57	MG	1A	3501	1/1	0.85	0.22	65,65,65,65	0
57	MG	2A	3168	1/1	0.85	0.15	50,50,50,50	0
57	MG	2A	3145	1/1	0.85	0.14	48,48,48,48	0
57	MG	1A	3784	1/1	0.85	0.21	28,28,28,28	0
57	MG	1a	3012	1/1	0.85	0.13	45,45,45,45	0
57	MG	2A	3241	1/1	0.85	0.40	54,54,54,54	0
57	MG	2A	3248	1/1	0.85	0.20	40,40,40,40	0
57	MG	2A	3429	1/1	0.85	0.23	55,55,55,55	0
57	MG	2A	3556	1/1	0.85	0.14	58,58,58,58	0
57	MG	1A	3974	1/1	0.85	0.12	54,54,54,54	0
57	MG	2a	3160	1/1	0.85	0.22	55,55,55,55	0
57	MG	2a	3079	1/1	0.85	0.29	61,61,61,61	0
57	MG	2A	3361	1/1	0.85	0.15	52,52,52,52	0
57	MG	2A	3039	1/1	0.85	0.14	28,28,28,28	0
57	MG	1A	3567	1/1	0.85	0.09	46,46,46,46	0
57	MG	1A	3560	1/1	0.85	0.21	55,55,55,55	0
57	MG	1A	3262	1/1	0.85	0.30	56,56,56,56	0
57	MG	2A	3129	1/1	0.85	0.08	48,48,48,48	0
57	MG	2A	3504	1/1	0.85	0.23	48,48,48,48	0
57	MG	1a	3163	1/1	0.85	0.17	64,64,64,64	0
57	MG	2a	3172	1/1	0.85	0.23	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	3544	1/1	0.85	0.12	43,43,43,43	0
57	MG	2A	3053	1/1	0.85	0.23	66,66,66,66	0
57	MG	1a	3132	1/1	0.85	0.16	53,53,53,53	0
57	MG	1a	3122	1/1	0.86	0.15	53,53,53,53	0
57	MG	2A	3714	1/1	0.86	0.17	42,42,42,42	0
57	MG	1A	3376	1/1	0.86	0.20	46,46,46,46	0
57	MG	2a	3148	1/1	0.86	0.12	63,63,63,63	0
57	MG	1A	3353	1/1	0.86	0.17	36,36,36,36	0
57	MG	2a	3277	1/1	0.86	0.18	56,56,56,56	0
57	MG	1a	3050	1/1	0.86	0.24	56,56,56,56	0
57	MG	1a	3204	1/1	0.86	0.22	71,71,71,71	0
57	MG	1A	3995	1/1	0.86	0.14	61,61,61,61	0
57	MG	2A	3560	1/1	0.86	0.17	60,60,60,60	0
57	MG	2A	3224	1/1	0.86	0.16	51,51,51,51	0
57	MG	1A	3435	1/1	0.86	0.16	60,60,60,60	0
57	MG	1A	4231	1/1	0.86	0.15	37,37,37,37	0
57	MG	2a	3207	1/1	0.86	0.10	53,53,53,53	0
57	MG	2a	3003	1/1	0.86	0.10	53,53,53,53	0
57	MG	2A	3474	1/1	0.86	0.20	51,51,51,51	0
57	MG	1A	4139	1/1	0.86	0.07	42,42,42,42	0
57	MG	1A	3702	1/1	0.86	0.17	54,54,54,54	0
57	MG	1A	3747	1/1	0.86	0.09	55,55,55,55	0
57	MG	2A	3785	1/1	0.86	0.20	58,58,58,58	0
57	MG	2A	3194	1/1	0.86	0.12	49,49,49,49	0
57	MG	1A	4168	1/1	0.86	0.10	56,56,56,56	0
57	MG	1A	3348	1/1	0.86	0.25	40,40,40,40	0
57	MG	1A	3485	1/1	0.86	0.20	37,37,37,37	0
57	MG	1A	3917	1/1	0.86	0.13	41,41,41,41	0
57	MG	2A	3512	1/1	0.86	0.22	49,49,49,49	0
57	MG	2A	3104	1/1	0.86	0.25	54,54,54,54	0
57	MG	2a	3159	1/1	0.86	0.13	48,48,48,48	0
57	MG	2A	3676	1/1	0.86	0.12	56,56,56,56	0
57	MG	2A	3300	1/1	0.86	0.10	58,58,58,58	0
57	MG	1A	3991	1/1	0.86	0.51	50,50,50,50	0
57	MG	1A	3525	1/1	0.86	0.20	41,41,41,41	0
57	MG	2a	3128	1/1	0.86	0.24	72,72,72,72	0
57	MG	2A	3178	1/1	0.86	0.21	69,69,69,69	0
57	MG	2A	3913	1/1	0.86	0.13	53,53,53,53	0
57	MG	2a	3067	1/1	0.86	0.11	54,54,54,54	0
57	MG	2A	3296	1/1	0.86	0.23	63,63,63,63	0
57	MG	1a	3233	1/1	0.86	0.15	46,46,46,46	0
57	MG	2A	3494	1/1	0.86	0.10	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	2A	3100	1/1	0.86	0.24	56,56,56,56	0
57	MG	1A	4025	1/1	0.86	0.11	36,36,36,36	0
57	MG	2A	3784	1/1	0.86	0.11	42,42,42,42	0
57	MG	1a	3117	1/1	0.86	0.17	55,55,55,55	0
57	MG	1A	3953	1/1	0.86	0.09	54,54,54,54	0
57	MG	2A	3173	1/1	0.86	0.18	54,54,54,54	0
57	MG	1A	4127	1/1	0.86	0.12	60,60,60,60	0
57	MG	1a	3252	1/1	0.86	0.11	53,53,53,53	0
57	MG	2a	3262	1/1	0.86	0.06	66,66,66,66	0
57	MG	1A	3510	1/1	0.86	0.20	46,46,46,46	0
57	MG	2A	3933	1/1	0.86	0.11	49,49,49,49	0
57	MG	2A	3232	1/1	0.86	0.46	42,42,42,42	0
57	MG	1A	3468	1/1	0.86	0.15	52,52,52,52	0
57	MG	1A	3152	1/1	0.86	0.22	37,37,37,37	0
57	MG	2A	3749	1/1	0.86	0.17	46,46,46,46	0
57	MG	1A	3092	1/1	0.86	0.27	43,43,43,43	0
57	MG	1A	3423	1/1	0.86	0.26	37,37,37,37	0
57	MG	2a	3217	1/1	0.86	0.11	57,57,57,57	0
57	MG	2A	3799	1/1	0.86	0.15	50,50,50,50	0
57	MG	2a	3034	1/1	0.86	0.17	54,54,54,54	0
57	MG	1A	3384	1/1	0.86	0.25	55,55,55,55	0
57	MG	2A	3162	1/1	0.86	0.24	47,47,47,47	0
57	MG	2A	3378	1/1	0.86	0.18	51,51,51,51	0
57	MG	1A	3201	1/1	0.86	0.19	44,44,44,44	0
57	MG	1A	3469	1/1	0.86	0.17	44,44,44,44	0
57	MG	2a	3267	1/1	0.86	0.23	61,61,61,61	0
57	MG	1A	3267	1/1	0.86	0.34	32,32,32,32	0
57	MG	2A	3252	1/1	0.86	0.39	59,59,59,59	0
57	MG	1a	3004	1/1	0.86	0.10	50,50,50,50	0
57	MG	2A	3886	1/1	0.86	0.17	65,65,65,65	0
57	MG	1A	4181	1/1	0.86	0.09	46,46,46,46	0
57	MG	2a	3121	1/1	0.86	0.13	58,58,58,58	0
57	MG	1A	3422	1/1	0.86	0.37	63,63,63,63	0
57	MG	2a	3185	1/1	0.86	0.40	65,65,65,65	0
57	MG	1a	3128	1/1	0.86	0.17	37,37,37,37	0
57	MG	1A	3848	1/1	0.86	0.13	38,38,38,38	0
57	MG	2a	3001	1/1	0.86	0.13	46,46,46,46	0
57	MG	1a	3121	1/1	0.86	0.16	60,60,60,60	0
57	MG	1A	3346	1/1	0.86	0.12	48,48,48,48	0
57	MG	2a	3191	1/1	0.86	0.10	74,74,74,74	0
57	MG	2A	3264	1/1	0.87	0.39	70,70,70,70	0
57	MG	1A	3306	1/1	0.87	0.10	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	4092	1/1	0.87	0.08	55,55,55,55	0
57	MG	2A	3702	1/1	0.87	0.14	38,38,38,38	0
57	MG	2A	3790	1/1	0.87	0.08	50,50,50,50	0
57	MG	2A	3373	1/1	0.87	0.21	57,57,57,57	0
57	MG	2A	3613	1/1	0.87	0.18	32,32,32,32	0
57	MG	2A	3005	1/1	0.87	0.27	55,55,55,55	0
57	MG	2A	3472	1/1	0.87	0.16	61,61,61,61	0
57	MG	2A	3805	1/1	0.87	0.16	61,61,61,61	0
57	MG	1a	3131	1/1	0.87	0.14	45,45,45,45	0
57	MG	2A	3301	1/1	0.87	0.29	60,60,60,60	0
57	MG	2A	3201	1/1	0.87	0.29	48,48,48,48	0
57	MG	1A	3248	1/1	0.87	0.12	45,45,45,45	0
57	MG	1A	3684	1/1	0.87	0.27	49,49,49,49	0
57	MG	1A	3936	1/1	0.87	0.24	16,16,16,16	0
57	MG	1A	3443	1/1	0.87	0.17	50,50,50,50	0
57	MG	1A	3551	1/1	0.87	0.13	45,45,45,45	0
57	MG	1A	3943	1/1	0.87	0.12	50,50,50,50	0
57	MG	1A	3861	1/1	0.87	0.23	18,18,18,18	0
57	MG	2A	3673	1/1	0.87	0.18	55,55,55,55	0
57	MG	2A	3122	1/1	0.87	0.17	46,46,46,46	0
57	MG	2A	3759	1/1	0.87	0.16	40,40,40,40	0
57	MG	1A	3139	1/1	0.87	0.13	26,26,26,26	0
57	MG	2A	3413	1/1	0.87	0.16	60,60,60,60	0
57	MG	1a	3227	1/1	0.87	0.10	60,60,60,60	0
57	MG	1A	4066	1/1	0.87	0.07	48,48,48,48	0
57	MG	2A	3748	1/1	0.87	0.17	65,65,65,65	0
57	MG	2A	3539	1/1	0.87	0.47	54,54,54,54	0
57	MG	2a	3072	1/1	0.87	0.17	54,54,54,54	0
57	MG	1a	3023	1/1	0.87	0.15	56,56,56,56	0
57	MG	2a	3109	1/1	0.87	0.21	51,51,51,51	0
57	MG	2a	3229	1/1	0.87	0.14	54,54,54,54	0
57	MG	1A	3479	1/1	0.87	0.16	32,32,32,32	0
57	MG	2A	3303	1/1	0.87	0.23	58,58,58,58	0
57	MG	2A	3004	1/1	0.87	0.17	43,43,43,43	0
57	MG	1A	3446	1/1	0.87	0.11	34,34,34,34	0
57	MG	1A	3776	1/1	0.87	0.12	36,36,36,36	0
57	MG	1A	4024	1/1	0.87	0.14	39,39,39,39	0
57	MG	1A	3916	1/1	0.87	0.09	47,47,47,47	0
57	MG	2a	3226	1/1	0.87	0.09	64,64,64,64	0
57	MG	2A	3446	1/1	0.87	0.21	44,44,44,44	0
57	MG	2A	3307	1/1	0.87	0.20	64,64,64,64	0
57	MG	1a	3024	1/1	0.87	0.18	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	1a	3030	1/1	0.87	0.14	46,46,46,46	0
57	MG	2A	3177	1/1	0.87	0.10	46,46,46,46	0
57	MG	1A	3323	1/1	0.87	0.16	36,36,36,36	0
57	MG	1A	4169	1/1	0.87	0.14	48,48,48,48	0
57	MG	2A	3237	1/1	0.87	0.23	39,39,39,39	0
57	MG	2A	3481	1/1	0.87	0.25	44,44,44,44	0
57	MG	1A	3356	1/1	0.87	0.18	54,54,54,54	0
57	MG	2A	3037	1/1	0.87	0.17	26,26,26,26	0
57	MG	2A	3217	1/1	0.87	0.24	52,52,52,52	0
57	MG	1A	3795	1/1	0.87	0.26	35,35,35,35	0
57	MG	1A	3652	1/1	0.87	0.61	62,62,62,62	0
57	MG	1A	3397	1/1	0.87	0.12	37,37,37,37	0
57	MG	1A	3534	1/1	0.87	0.17	42,42,42,42	0
57	MG	1A	3668	1/1	0.87	0.26	43,43,43,43	0
57	MG	2A	3764	1/1	0.87	0.13	67,67,67,67	0
57	MG	1a	3034	1/1	0.87	0.22	23,23,23,23	0
57	MG	1A	3317	1/1	0.87	0.14	27,27,27,27	0
57	MG	1A	4026	1/1	0.87	0.13	20,20,20,20	0
57	MG	2A	3399	1/1	0.87	0.24	58,58,58,58	0
57	MG	1a	3205	1/1	0.87	0.08	51,51,51,51	0
57	MG	2A	3422	1/1	0.87	0.12	61,61,61,61	0
57	MG	1A	3307	1/1	0.87	0.18	31,31,31,31	0
57	MG	1A	4201	1/1	0.87	0.17	42,42,42,42	0
57	MG	1A	4230	1/1	0.87	0.23	39,39,39,39	0
57	MG	1A	4218	1/1	0.87	0.17	36,36,36,36	0
57	MG	1A	3429	1/1	0.87	0.20	38,38,38,38	0
57	MG	2a	3179	1/1	0.87	0.22	55,55,55,55	0
57	MG	2A	3700	1/1	0.87	0.15	51,51,51,51	0
57	MG	2A	3286	1/1	0.87	0.16	48,48,48,48	0
57	MG	2A	3789	1/1	0.87	0.07	45,45,45,45	0
57	MG	1A	3706	1/1	0.87	0.28	51,51,51,51	0
57	MG	2A	3750	1/1	0.87	0.19	49,49,49,49	0
57	MG	2a	3181	1/1	0.87	0.13	64,64,64,64	0
57	MG	2a	3131	1/1	0.87	0.12	43,43,43,43	0
57	MG	1A	3234	1/1	0.87	0.18	36,36,36,36	0
57	MG	2a	3256	1/1	0.87	0.09	62,62,62,62	0
57	MG	1A	3875	1/1	0.87	0.14	45,45,45,45	0
57	MG	2A	3819	1/1	0.87	0.17	61,61,61,61	0
57	MG	1A	3527	1/1	0.87	0.24	41,41,41,41	0
57	MG	2a	3056	1/1	0.87	0.18	57,57,57,57	0
57	MG	2A	3289	1/1	0.87	0.13	50,50,50,50	0
57	MG	1A	3159	1/1	0.88	0.30	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	3460	1/1	0.88	0.10	59,59,59,59	0
57	MG	1A	3890	1/1	0.88	0.13	57,57,57,57	0
57	MG	1A	3507	1/1	0.88	0.14	52,52,52,52	0
57	MG	1A	3828	1/1	0.88	0.18	27,27,27,27	0
57	MG	2A	3624	1/1	0.88	0.18	41,41,41,41	0
57	MG	2A	3930	1/1	0.88	0.12	30,30,30,30	0
57	MG	1A	3613	1/1	0.88	0.20	40,40,40,40	0
57	MG	1A	4012	1/1	0.88	0.16	31,31,31,31	0
57	MG	1A	3779	1/1	0.88	0.15	25,25,25,25	0
57	MG	2A	3636	1/1	0.88	0.12	32,32,32,32	0
57	MG	2a	3012	1/1	0.88	0.21	51,51,51,51	0
57	MG	2A	3228	1/1	0.88	0.17	52,52,52,52	0
57	MG	1A	3646	1/1	0.88	0.20	47,47,47,47	0
57	MG	2A	3136	1/1	0.88	0.21	56,56,56,56	0
57	MG	2a	3061	1/1	0.88	0.20	73,73,73,73	0
57	MG	2A	3072	1/1	0.88	0.16	30,30,30,30	0
57	MG	2a	3213	1/1	0.88	0.11	73,73,73,73	0
57	MG	2A	3048	1/1	0.88	0.12	58,58,58,58	0
57	MG	1a	3174	1/1	0.88	0.13	49,49,49,49	0
57	MG	2A	3664	1/1	0.88	0.18	55,55,55,55	0
57	MG	1A	3574	1/1	0.88	0.28	51,51,51,51	0
57	MG	2A	3364	1/1	0.88	0.11	52,52,52,52	0
57	MG	2A	3014	1/1	0.88	0.19	35,35,35,35	0
57	MG	1a	3073	1/1	0.88	0.15	45,45,45,45	0
57	MG	2A	3561	1/1	0.88	0.11	62,62,62,62	0
57	MG	2A	3089	1/1	0.88	0.16	49,49,49,49	0
57	MG	2A	3559	1/1	0.88	0.20	62,62,62,62	0
57	MG	2A	3530	1/1	0.88	0.19	67,67,67,67	0
57	MG	1A	4104	1/1	0.88	0.13	55,55,55,55	0
57	MG	2a	3223	1/1	0.88	0.18	40,40,40,40	0
57	MG	1A	4040	1/1	0.88	0.18	48,48,48,48	0
57	MG	2a	3247	1/1	0.88	0.17	56,56,56,56	0
57	MG	2A	3616	1/1	0.88	0.21	41,41,41,41	0
57	MG	1A	3178	1/1	0.88	0.21	52,52,52,52	0
57	MG	1a	3243	1/1	0.88	0.30	56,56,56,56	0
57	MG	1a	3170	1/1	0.88	0.17	64,64,64,64	0
57	MG	2A	3568	1/1	0.88	0.21	42,42,42,42	0
57	MG	1A	4286	1/1	0.88	0.19	58,58,58,58	0
57	MG	1a	3249	1/1	0.88	0.13	59,59,59,59	0
57	MG	1A	3832	1/1	0.88	0.14	60,60,60,60	0
57	MG	2A	3815	1/1	0.88	0.10	51,51,51,51	0
57	MG	1A	4228	1/1	0.88	0.15	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	2A	3459	1/1	0.88	0.20	44,44,44,44	0
57	MG	1A	3333	1/1	0.88	0.18	53,53,53,53	0
57	MG	2a	3018	1/1	0.88	0.12	54,54,54,54	0
57	MG	1a	3229	1/1	0.88	0.10	56,56,56,56	0
57	MG	2a	3071	1/1	0.88	0.33	66,66,66,66	0
57	MG	1A	4088	1/1	0.88	0.08	45,45,45,45	0
57	MG	2a	3269	1/1	0.88	0.16	65,65,65,65	0
57	MG	2A	3144	1/1	0.88	0.20	30,30,30,30	0
57	MG	2A	3964	1/1	0.88	0.08	64,64,64,64	0
57	MG	1A	4067	1/1	0.88	0.10	48,48,48,48	0
57	MG	1A	3247	1/1	0.88	0.10	60,60,60,60	0
57	MG	2A	3284	1/1	0.88	0.20	50,50,50,50	0
57	MG	1A	3606	1/1	0.88	0.31	59,59,59,59	0
57	MG	2A	3753	1/1	0.88	0.09	73,73,73,73	0
57	MG	1A	4223	1/1	0.88	0.14	42,42,42,42	0
57	MG	2a	3046	1/1	0.88	0.34	59,59,59,59	0
57	MG	1A	3994	1/1	0.88	0.14	64,64,64,64	0
57	MG	2A	3230	1/1	0.88	0.10	64,64,64,64	0
57	MG	1A	4134	1/1	0.88	0.14	25,25,25,25	0
57	MG	2a	3180	1/1	0.88	0.14	60,60,60,60	0
57	MG	2a	3244	1/1	0.88	0.07	56,56,56,56	0
57	MG	2A	3205	1/1	0.88	0.17	52,52,52,52	0
57	MG	2A	3101	1/1	0.88	0.12	40,40,40,40	0
57	MG	2A	3687	1/1	0.88	0.20	41,41,41,41	0
57	MG	1a	3232	1/1	0.88	0.12	39,39,39,39	0
57	MG	1A	3609	1/1	0.88	0.14	56,56,56,56	0
57	MG	2A	3690	1/1	0.88	0.13	55,55,55,55	0
57	MG	2A	3214	1/1	0.88	0.20	52,52,52,52	0
57	MG	1A	3273	1/1	0.88	0.16	63,63,63,63	0
57	MG	2A	3480	1/1	0.88	0.18	57,57,57,57	0
57	MG	1A	3308	1/1	0.88	0.18	51,51,51,51	0
57	MG	2A	3240	1/1	0.88	0.13	34,34,34,34	0
57	MG	2A	3203	1/1	0.88	0.18	55,55,55,55	0
57	MG	2a	3162	1/1	0.88	0.25	51,51,51,51	0
57	MG	1A	4022	1/1	0.88	0.14	62,62,62,62	0
57	MG	1a	3041	1/1	0.88	0.16	58,58,58,58	0
57	MG	2a	3117	1/1	0.88	0.18	69,69,69,69	0
57	MG	2A	3260	1/1	0.88	0.09	52,52,52,52	0
57	MG	2A	3841	1/1	0.88	0.20	63,63,63,63	0
57	MG	2A	3132	1/1	0.88	0.13	61,61,61,61	0
57	MG	2A	3475	1/1	0.88	0.18	51,51,51,51	0
57	MG	1A	3657	1/1	0.88	0.19	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	3421	1/1	0.88	0.20	46,46,46,46	0
57	MG	2A	3270	1/1	0.88	0.14	48,48,48,48	0
57	MG	1A	3878	1/1	0.88	0.19	50,50,50,50	0
57	MG	2A	3717	1/1	0.88	0.11	70,70,70,70	0
57	MG	2A	3326	1/1	0.88	0.15	57,57,57,57	0
57	MG	2A	3546	1/1	0.88	0.12	61,61,61,61	0
57	MG	2A	3533	1/1	0.88	0.18	56,56,56,56	0
57	MG	1a	3251	1/1	0.88	0.13	69,69,69,69	0
57	MG	2a	3184	1/1	0.88	0.15	68,68,68,68	0
57	MG	2a	3169	1/1	0.88	0.18	40,40,40,40	0
57	MG	2A	3135	1/1	0.89	0.10	63,63,63,63	0
57	MG	2A	3686	1/1	0.89	0.10	42,42,42,42	0
57	MG	2A	3121	1/1	0.89	0.21	45,45,45,45	0
57	MG	2a	3105	1/1	0.89	0.17	58,58,58,58	0
57	MG	1A	4052	1/1	0.89	0.17	39,39,39,39	0
57	MG	1A	4005	1/1	0.89	0.20	47,47,47,47	0
57	MG	2A	3047	1/1	0.89	0.15	52,52,52,52	0
57	MG	1a	3161	1/1	0.89	0.12	30,30,30,30	0
57	MG	2A	3340	1/1	0.89	0.18	48,48,48,48	0
57	MG	2A	3015	1/1	0.89	0.16	39,39,39,39	0
57	MG	1A	3252	1/1	0.89	0.27	29,29,29,29	0
57	MG	2a	3204	1/1	0.89	0.14	65,65,65,65	0
57	MG	1A	3876	1/1	0.89	0.10	45,45,45,45	0
57	MG	2A	3925	1/1	0.89	0.16	60,60,60,60	0
57	MG	2A	3665	1/1	0.89	0.14	47,47,47,47	0
57	MG	1A	3383	1/1	0.89	0.18	53,53,53,53	0
57	MG	2A	3011	1/1	0.89	0.18	39,39,39,39	0
57	MG	2a	3141	1/1	0.89	0.16	45,45,45,45	0
57	MG	2A	3735	1/1	0.89	0.10	46,46,46,46	0
57	MG	2a	3015	1/1	0.89	0.10	53,53,53,53	0
57	MG	2a	3214	1/1	0.89	0.19	71,71,71,71	0
57	MG	2A	3610	1/1	0.89	0.14	48,48,48,48	0
57	MG	2A	3034	1/1	0.89	0.12	53,53,53,53	0
57	MG	1A	3709	1/1	0.89	0.14	37,37,37,37	0
57	MG	2A	3006	1/1	0.89	0.27	51,51,51,51	0
57	MG	1A	3377	1/1	0.89	0.29	37,37,37,37	0
57	MG	2A	3854	1/1	0.89	0.12	48,48,48,48	0
57	MG	2A	3210	1/1	0.89	0.12	62,62,62,62	0
57	MG	2A	3733	1/1	0.89	0.12	51,51,51,51	0
57	MG	1A	3786	1/1	0.89	0.11	21,21,21,21	0
57	MG	2A	3491	1/1	0.89	0.17	58,58,58,58	0
57	MG	2A	3148	1/1	0.89	0.15	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	4013	1/1	0.89	0.48	39,39,39,39	0
57	MG	2A	3302	1/1	0.89	0.18	51,51,51,51	0
57	MG	2a	3083	1/1	0.89	0.20	53,53,53,53	0
57	MG	1A	3970	1/1	0.89	0.11	44,44,44,44	0
57	MG	2A	3842	1/1	0.89	0.19	59,59,59,59	0
57	MG	1A	3460	1/1	0.89	0.09	48,48,48,48	0
57	MG	1A	3971	1/1	0.89	0.13	48,48,48,48	0
57	MG	2a	3278	1/1	0.89	0.10	57,57,57,57	0
57	MG	2A	3548	1/1	0.89	0.14	64,64,64,64	0
57	MG	2A	3736	1/1	0.89	0.09	61,61,61,61	0
57	MG	1A	3573	1/1	0.89	0.12	54,54,54,54	0
57	MG	1A	3224	1/1	0.89	0.19	56,56,56,56	0
57	MG	1A	3648	1/1	0.89	0.17	37,37,37,37	0
57	MG	2A	3137	1/1	0.89	0.13	41,41,41,41	0
57	MG	2A	3703	1/1	0.89	0.16	34,34,34,34	0
57	MG	1A	3163	1/1	0.89	0.20	36,36,36,36	0
57	MG	1a	3250	1/1	0.89	0.09	65,65,65,65	0
57	MG	2A	3375	1/1	0.89	0.22	56,56,56,56	0
57	MG	1a	3143	1/1	0.89	0.20	53,53,53,53	0
57	MG	1a	3156	1/1	0.89	0.11	46,46,46,46	0
57	MG	1A	4100	1/1	0.89	0.11	36,36,36,36	0
57	MG	2A	3726	1/1	0.89	0.17	57,57,57,57	0
57	MG	1A	3332	1/1	0.89	0.20	43,43,43,43	0
57	MG	1a	3006	1/1	0.89	0.18	47,47,47,47	0
57	MG	2a	3057	1/1	0.89	0.15	62,62,62,62	0
57	MG	1a	3055	1/1	0.89	0.11	51,51,51,51	0
57	MG	1A	4072	1/1	0.89	0.17	38,38,38,38	0
57	MG	1A	3462	1/1	0.89	0.35	50,50,50,50	0
57	MG	2A	3227	1/1	0.89	0.08	52,52,52,52	0
57	MG	2A	3514	1/1	0.89	0.29	37,37,37,37	0
57	MG	1A	3264	1/1	0.89	0.19	49,49,49,49	0
57	MG	1A	3269	1/1	0.89	0.14	50,50,50,50	0
57	MG	1A	3583	1/1	0.89	0.21	32,32,32,32	0
57	MG	2A	3643	1/1	0.89	0.19	40,40,40,40	0
57	MG	1A	3535	1/1	0.89	0.11	32,32,32,32	0
57	MG	1A	3664	1/1	0.89	0.26	40,40,40,40	0
57	MG	2A	3384	1/1	0.89	0.48	52,52,52,52	0
57	MG	2A	3108	1/1	0.89	0.10	51,51,51,51	0
57	MG	2A	3314	1/1	0.89	0.11	42,42,42,42	0
57	MG	1A	3605	1/1	0.89	0.16	26,26,26,26	0
57	MG	1A	3378	1/1	0.89	0.21	35,35,35,35	0
57	MG	2a	3016	1/1	0.89	0.10	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	2A	3450	1/1	0.89	0.13	47,47,47,47	0
57	MG	2A	3342	1/1	0.89	0.24	61,61,61,61	0
57	MG	1A	3235	1/1	0.89	0.20	36,36,36,36	0
57	MG	2A	3198	1/1	0.89	0.14	62,62,62,62	0
57	MG	1A	4029	1/1	0.89	0.18	37,37,37,37	0
57	MG	1A	3320	1/1	0.89	0.22	35,35,35,35	0
57	MG	1a	3145	1/1	0.89	0.17	52,52,52,52	0
57	MG	1A	4074	1/1	0.89	0.20	44,44,44,44	0
57	MG	1A	3584	1/1	0.89	0.15	47,47,47,47	0
57	MG	1A	3611	1/1	0.89	0.14	57,57,57,57	0
57	MG	2A	3408	1/1	0.89	0.29	57,57,57,57	0
57	MG	1A	3667	1/1	0.89	0.37	37,37,37,37	0
57	MG	1A	4211	1/1	0.89	0.11	36,36,36,36	0
57	MG	2a	3095	1/1	0.89	0.11	49,49,49,49	0
57	MG	1a	3018	1/1	0.89	0.16	44,44,44,44	0
57	MG	1A	4186	1/1	0.89	0.11	55,55,55,55	0
57	MG	1a	3150	1/1	0.89	0.16	45,45,45,45	0
57	MG	1A	3610	1/1	0.89	0.22	48,48,48,48	0
57	MG	2A	3060	1/1	0.89	0.28	63,63,63,63	0
57	MG	1A	4154	1/1	0.89	0.14	31,31,31,31	0
57	MG	2A	3258	1/1	0.89	0.49	64,64,64,64	0
57	MG	1A	4060	1/1	0.89	0.20	37,37,37,37	0
57	MG	1A	3946	1/1	0.89	0.09	29,29,29,29	0
57	MG	1A	4081	1/1	0.89	0.13	44,44,44,44	0
57	MG	2A	3457	1/1	0.89	0.19	49,49,49,49	0
57	MG	2a	3266	1/1	0.89	0.27	52,52,52,52	0
57	MG	1A	3150	1/1	0.89	0.13	41,41,41,41	0
57	MG	2A	3825	1/1	0.89	0.14	31,31,31,31	0
57	MG	1A	3578	1/1	0.89	0.22	46,46,46,46	0
57	MG	1A	3881	1/1	0.89	0.17	20,20,20,20	0
57	MG	2A	3185	1/1	0.89	0.23	46,46,46,46	0
57	MG	1A	3158	1/1	0.89	0.19	30,30,30,30	0
57	MG	1A	3062	1/1	0.89	0.20	34,34,34,34	0
57	MG	2A	3543	1/1	0.89	0.14	47,47,47,47	0
57	MG	1A	3593	1/1	0.89	0.33	44,44,44,44	0
57	MG	1A	3874	1/1	0.89	0.14	25,25,25,25	0
57	MG	1a	3234	1/1	0.89	0.13	49,49,49,49	0
57	MG	1A	3597	1/1	0.89	0.17	38,38,38,38	0
57	MG	2A	3085	1/1	0.89	0.17	60,60,60,60	0
57	MG	2A	3276	1/1	0.89	0.12	48,48,48,48	0
57	MG	1A	3424	1/1	0.89	0.18	66,66,66,66	0
57	MG	2A	3892	1/1	0.89	0.09	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	2A	3334	1/1	0.89	0.14	46,46,46,46	0
57	MG	2A	3657	1/1	0.89	0.22	55,55,55,55	0
57	MG	1A	3427	1/1	0.89	0.12	17,17,17,17	0
57	MG	1A	3852	1/1	0.89	0.09	47,47,47,47	0
57	MG	2A	3187	1/1	0.89	0.11	55,55,55,55	0
57	MG	2a	3004	1/1	0.90	0.17	51,51,51,51	0
57	MG	1A	4267	1/1	0.90	0.15	60,60,60,60	0
57	MG	1A	3540	1/1	0.90	0.17	53,53,53,53	0
57	MG	2A	3929	1/1	0.90	0.27	56,56,56,56	0
57	MG	2A	3603	1/1	0.90	0.14	49,49,49,49	0
57	MG	1A	3195	1/1	0.90	0.16	46,46,46,46	0
57	MG	1A	4069	1/1	0.90	0.09	41,41,41,41	0
57	MG	1a	3108	1/1	0.90	0.10	59,59,59,59	0
57	MG	1A	3858	1/1	0.90	0.22	37,37,37,37	0
57	MG	1A	3904	1/1	0.90	0.16	28,28,28,28	0
57	MG	2A	3095	1/1	0.90	0.37	42,42,42,42	0
57	MG	2A	3756	1/1	0.90	0.11	55,55,55,55	0
57	MG	2A	3701	1/1	0.90	0.10	51,51,51,51	0
57	MG	2A	3771	1/1	0.90	0.26	72,72,72,72	0
57	MG	1A	3408	1/1	0.90	0.15	32,32,32,32	0
57	MG	1A	3686	1/1	0.90	0.13	42,42,42,42	0
57	MG	1A	4170	1/1	0.90	0.12	46,46,46,46	0
57	MG	1A	3499	1/1	0.90	0.18	38,38,38,38	0
57	MG	1A	4083	1/1	0.90	0.08	41,41,41,41	0
57	MG	2A	3555	1/1	0.90	0.23	46,46,46,46	0
57	MG	1A	3879	1/1	0.90	0.13	41,41,41,41	0
57	MG	2a	3170	1/1	0.90	0.11	44,44,44,44	0
57	MG	1a	3182	1/1	0.90	0.18	60,60,60,60	0
57	MG	2A	3455	1/1	0.90	0.12	51,51,51,51	0
57	MG	1A	4283	1/1	0.90	0.12	37,37,37,37	0
57	MG	2a	3273	1/1	0.90	0.13	60,60,60,60	0
57	MG	1a	3039	1/1	0.90	0.25	47,47,47,47	0
57	MG	2A	3243	1/1	0.90	0.19	57,57,57,57	0
57	MG	1a	3236	1/1	0.90	0.18	65,65,65,65	0
57	MG	1A	3906	1/1	0.90	0.21	27,27,27,27	0
57	MG	2a	3173	1/1	0.90	0.14	47,47,47,47	0
57	MG	2A	3018	1/1	0.90	0.22	49,49,49,49	0
57	MG	2A	3605	1/1	0.90	0.14	48,48,48,48	0
57	MG	1A	3630	1/1	0.90	0.12	21,21,21,21	0
57	MG	2a	3281	1/1	0.90	0.14	59,59,59,59	0
57	MG	1A	4105	1/1	0.90	0.31	38,38,38,38	0
57	MG	1A	3324	1/1	0.90	0.23	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	3821	1/1	0.90	0.20	60,60,60,60	0
57	MG	1A	3211	1/1	0.90	0.28	48,48,48,48	0
57	MG	1A	3214	1/1	0.90	0.19	34,34,34,34	0
57	MG	2A	3077	1/1	0.90	0.17	49,49,49,49	0
57	MG	1A	3176	1/1	0.90	0.14	36,36,36,36	0
57	MG	1A	4149	1/1	0.90	0.07	45,45,45,45	0
57	MG	1a	3076	1/1	0.90	0.13	58,58,58,58	0
57	MG	1A	3731	1/1	0.90	0.19	29,29,29,29	0
57	MG	1A	3853	1/1	0.90	0.20	59,59,59,59	0
57	MG	2a	3069	1/1	0.90	0.09	57,57,57,57	0
57	MG	2A	3127	1/1	0.90	0.15	66,66,66,66	0
57	MG	2A	3872	1/1	0.90	0.14	51,51,51,51	0
57	MG	1A	3294	1/1	0.90	0.48	39,39,39,39	0
57	MG	2A	3036	1/1	0.90	0.15	51,51,51,51	0
57	MG	2A	3538	1/1	0.90	0.09	48,48,48,48	0
57	MG	1A	3412	1/1	0.90	0.14	40,40,40,40	0
57	MG	2A	3418	1/1	0.90	0.16	50,50,50,50	0
57	MG	1A	3232	1/1	0.90	0.26	29,29,29,29	0
57	MG	1A	3666	1/1	0.90	0.27	27,27,27,27	0
57	MG	1a	3231	1/1	0.90	0.09	57,57,57,57	0
57	MG	1A	4244	1/1	0.90	0.15	35,35,35,35	0
57	MG	1A	3290	1/1	0.90	0.14	32,32,32,32	0
57	MG	2A	3271	1/1	0.90	0.23	45,45,45,45	0
57	MG	1A	3484	1/1	0.90	0.49	45,45,45,45	0
57	MG	2a	3232	1/1	0.90	0.10	70,70,70,70	0
57	MG	2a	3082	1/1	0.90	0.12	49,49,49,49	0
57	MG	2A	3516	1/1	0.90	0.11	52,52,52,52	0
57	MG	1A	4131	1/1	0.90	0.14	28,28,28,28	0
57	MG	1A	3493	1/1	0.90	0.20	44,44,44,44	0
57	MG	1a	3104	1/1	0.90	0.13	51,51,51,51	0
57	MG	2A	3281	1/1	0.90	0.22	53,53,53,53	0
57	MG	1A	4114	1/1	0.90	0.16	40,40,40,40	0
57	MG	2a	3086	1/1	0.90	0.15	60,60,60,60	0
57	MG	2A	3721	1/1	0.90	0.15	65,65,65,65	0
57	MG	2A	3238	1/1	0.90	0.34	46,46,46,46	0
57	MG	2a	3078	1/1	0.90	0.14	50,50,50,50	0
57	MG	1A	4070	1/1	0.90	0.12	39,39,39,39	0
57	MG	1A	3522	1/1	0.90	0.22	43,43,43,43	0
57	MG	1A	3698	1/1	0.90	0.20	50,50,50,50	0
57	MG	1A	3251	1/1	0.90	0.15	55,55,55,55	0
57	MG	2A	3415	1/1	0.90	0.11	55,55,55,55	0
57	MG	1A	4276	1/1	0.90	0.15	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	3218	1/1	0.90	0.09	57,57,57,57	0
57	MG	1A	3058	1/1	0.90	0.20	33,33,33,33	0
57	MG	1A	3302	1/1	0.90	0.34	29,29,29,29	0
57	MG	1A	3216	1/1	0.90	0.15	32,32,32,32	0
57	MG	1A	4297	1/1	0.90	0.24	47,47,47,47	0
57	MG	2A	3562	1/1	0.90	0.15	26,26,26,26	0
57	MG	1A	3350	1/1	0.90	0.18	41,41,41,41	0
57	MG	1A	3680	1/1	0.90	0.09	31,31,31,31	0
57	MG	1A	3138	1/1	0.90	0.20	29,29,29,29	0
57	MG	2A	3501	1/1	0.90	0.09	44,44,44,44	0
57	MG	1A	4294	1/1	0.90	0.12	40,40,40,40	0
57	MG	1a	3098	1/1	0.90	0.17	46,46,46,46	0
57	MG	2a	3063	1/1	0.90	0.36	63,63,63,63	0
57	MG	1A	4232	1/1	0.90	0.12	57,57,57,57	0
57	MG	2A	3316	1/1	0.90	0.15	44,44,44,44	0
57	MG	1A	3487	1/1	0.90	0.14	56,56,56,56	0
57	MG	2A	3961	1/1	0.90	0.12	53,53,53,53	0
57	MG	2A	3488	1/1	0.90	0.14	72,72,72,72	0
57	MG	2A	3345	1/1	0.90	0.34	66,66,66,66	0
57	MG	1A	4280	1/1	0.90	0.30	36,36,36,36	0
57	MG	1A	4019	1/1	0.90	0.19	43,43,43,43	0
57	MG	2A	3319	1/1	0.90	0.13	55,55,55,55	0
57	MG	1A	3413	1/1	0.90	0.21	37,37,37,37	0
57	MG	1A	3822	1/1	0.90	0.14	17,17,17,17	0
57	MG	2a	3161	1/1	0.90	0.15	62,62,62,62	0
57	MG	1A	3912	1/1	0.90	0.12	51,51,51,51	0
57	MG	1a	3072	1/1	0.90	0.15	43,43,43,43	0
57	MG	2a	3182	1/1	0.90	0.16	59,59,59,59	0
57	MG	1A	3166	1/1	0.90	0.11	39,39,39,39	0
57	MG	2A	3621	1/1	0.90	0.19	39,39,39,39	0
57	MG	1A	3730	1/1	0.90	0.14	49,49,49,49	0
57	MG	1A	3660	1/1	0.90	0.11	56,56,56,56	0
57	MG	2A	3139	1/1	0.90	0.13	40,40,40,40	0
57	MG	1a	3235	1/1	0.90	0.09	50,50,50,50	0
57	MG	2a	3019	1/1	0.90	0.13	51,51,51,51	0
57	MG	2A	3268	1/1	0.90	0.14	49,49,49,49	0
57	MG	2A	3204	1/1	0.90	0.17	44,44,44,44	0
57	MG	1a	3032	1/1	0.90	0.25	54,54,54,54	0
57	MG	1A	4263	1/1	0.90	0.15	24,24,24,24	0
57	MG	1A	3385	1/1	0.90	0.15	29,29,29,29	0
57	MG	1A	3590	1/1	0.90	0.16	46,46,46,46	0
57	MG	1a	3105	1/1	0.90	0.24	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	1a	3094	1/1	0.90	0.27	46,46,46,46	0
57	MG	1a	3082	1/1	0.90	0.13	48,48,48,48	0
57	MG	1A	3388	1/1	0.90	0.12	33,33,33,33	0
57	MG	2A	3693	1/1	0.90	0.16	50,50,50,50	0
57	MG	2A	3765	1/1	0.90	0.05	54,54,54,54	0
57	MG	1A	3585	1/1	0.90	0.16	53,53,53,53	0
57	MG	1a	3092	1/1	0.90	0.27	46,46,46,46	0
57	MG	2A	3030	1/1	0.90	0.25	54,54,54,54	0
57	MG	2A	3387	1/1	0.90	0.10	52,52,52,52	0
57	MG	1A	3143	1/1	0.90	0.11	36,36,36,36	0
57	MG	1A	3903	1/1	0.90	0.17	23,23,23,23	0
57	MG	2A	3050	1/1	0.90	0.12	48,48,48,48	0
57	MG	1A	4047	1/1	0.90	0.14	37,37,37,37	0
57	MG	1A	3230	1/1	0.90	0.18	49,49,49,49	0
57	MG	1A	3120	1/1	0.90	0.18	31,31,31,31	0
57	MG	2A	3288	1/1	0.90	0.11	54,54,54,54	0
57	MG	1a	3013	1/1	0.90	0.10	60,60,60,60	0
57	MG	2A	3552	1/1	0.90	0.13	41,41,41,41	0
57	MG	1A	4293	1/1	0.91	0.42	56,56,56,56	0
57	MG	1A	4295	1/1	0.91	0.23	46,46,46,46	0
57	MG	1A	3726	1/1	0.91	0.17	34,34,34,34	0
57	MG	2a	3068	1/1	0.91	0.08	67,67,67,67	0
57	MG	2A	3184	1/1	0.91	0.17	64,64,64,64	0
57	MG	2A	3727	1/1	0.91	0.12	62,62,62,62	0
57	MG	1A	4087	1/1	0.91	0.19	47,47,47,47	0
57	MG	2A	3274	1/1	0.91	0.13	44,44,44,44	0
57	MG	2A	3062	1/1	0.91	0.10	50,50,50,50	0
57	MG	2a	3242	1/1	0.91	0.13	42,42,42,42	0
57	MG	2A	3565	1/1	0.91	0.23	33,33,33,33	0
57	MG	2A	3832	1/1	0.91	0.10	50,50,50,50	0
57	MG	1A	3681	1/1	0.91	0.24	52,52,52,52	0
57	MG	1A	3237	1/1	0.91	0.21	31,31,31,31	0
57	MG	2A	3467	1/1	0.91	0.30	41,41,41,41	0
57	MG	1A	3239	1/1	0.91	0.29	50,50,50,50	0
57	MG	1A	3855	1/1	0.91	0.16	47,47,47,47	0
57	MG	2A	3699	1/1	0.91	0.15	36,36,36,36	0
57	MG	2a	3240	1/1	0.91	0.27	56,56,56,56	0
57	MG	1a	3172	1/1	0.91	0.14	54,54,54,54	0
57	MG	1A	3057	1/1	0.91	0.18	36,36,36,36	0
57	MG	1A	3311	1/1	0.91	0.22	33,33,33,33	0
57	MG	1A	3096	1/1	0.91	0.16	43,43,43,43	0
57	MG	1A	3794	1/1	0.91	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	3254	1/1	0.91	0.18	58,58,58,58	0
57	MG	1A	3167	1/1	0.91	0.20	19,19,19,19	0
57	MG	2A	3531	1/1	0.91	0.24	66,66,66,66	0
57	MG	2A	3046	1/1	0.91	0.28	46,46,46,46	0
57	MG	2a	3254	1/1	0.91	0.22	40,40,40,40	0
57	MG	2A	3212	1/1	0.91	0.12	57,57,57,57	0
57	MG	2A	3310	1/1	0.91	0.10	69,69,69,69	0
57	MG	2A	3510	1/1	0.91	0.21	52,52,52,52	0
57	MG	1A	4187	1/1	0.91	0.12	42,42,42,42	0
57	MG	1A	3084	1/1	0.91	0.27	29,29,29,29	0
57	MG	1A	3056	1/1	0.91	0.12	36,36,36,36	0
57	MG	2A	3195	1/1	0.91	0.16	57,57,57,57	0
57	MG	1A	3221	1/1	0.91	0.15	45,45,45,45	0
57	MG	1A	3335	1/1	0.91	0.16	30,30,30,30	0
57	MG	2A	3380	1/1	0.91	0.19	50,50,50,50	0
57	MG	2A	3401	1/1	0.91	0.18	54,54,54,54	0
57	MG	1A	4123	1/1	0.91	0.09	56,56,56,56	0
57	MG	2a	3156	1/1	0.91	0.16	52,52,52,52	0
57	MG	1A	3788	1/1	0.91	0.22	58,58,58,58	0
57	MG	1A	4095	1/1	0.91	0.13	45,45,45,45	0
57	MG	1A	3202	1/1	0.91	0.19	29,29,29,29	0
57	MG	1A	4085	1/1	0.91	0.14	21,21,21,21	0
57	MG	1a	3164	1/1	0.91	0.18	59,59,59,59	0
57	MG	2A	3485	1/1	0.91	0.16	49,49,49,49	0
57	MG	2A	3653	1/1	0.91	0.12	53,53,53,53	0
57	MG	2A	3876	1/1	0.91	0.11	55,55,55,55	0
57	MG	2A	3349	1/1	0.91	0.10	46,46,46,46	0
57	MG	2A	3379	1/1	0.91	0.18	59,59,59,59	0
57	MG	1A	3026	1/1	0.91	0.22	35,35,35,35	0
57	MG	1A	3289	1/1	0.91	0.19	35,35,35,35	0
57	MG	2A	3386	1/1	0.91	0.15	65,65,65,65	0
57	MG	2a	3021	1/1	0.91	0.30	67,67,67,67	0
57	MG	1A	4164	1/1	0.91	0.11	57,57,57,57	0
57	MG	1A	3470	1/1	0.91	0.16	38,38,38,38	0
57	MG	2a	3265	1/1	0.91	0.13	69,69,69,69	0
57	MG	2A	3836	1/1	0.91	0.14	46,46,46,46	0
57	MG	1a	3053	1/1	0.91	0.16	34,34,34,34	0
57	MG	1A	3002	1/1	0.91	0.13	41,41,41,41	0
57	MG	2a	3215	1/1	0.91	0.09	69,69,69,69	0
57	MG	2A	3881	1/1	0.91	0.08	47,47,47,47	0
57	MG	1A	3198	1/1	0.91	0.22	31,31,31,31	0
57	MG	2A	3233	1/1	0.91	0.12	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	3019	1/1	0.91	0.32	33,33,33,33	0
57	MG	1a	3031	1/1	0.91	0.18	49,49,49,49	0
57	MG	2A	3358	1/1	0.91	0.39	61,61,61,61	0
57	MG	1a	3062	1/1	0.91	0.20	61,61,61,61	0
57	MG	1A	4044	1/1	0.91	0.19	53,53,53,53	0
57	MG	2A	3357	1/1	0.91	0.16	56,56,56,56	0
57	MG	1A	4175	1/1	0.91	0.08	32,32,32,32	0
57	MG	2A	3632	1/1	0.91	0.15	31,31,31,31	0
57	MG	2A	3477	1/1	0.91	0.13	45,45,45,45	0
57	MG	1A	4250	1/1	0.91	0.13	44,44,44,44	0
57	MG	1A	3106	1/1	0.91	0.16	48,48,48,48	0
57	MG	2A	3863	1/1	0.91	0.10	58,58,58,58	0
57	MG	2a	3040	1/1	0.91	0.20	59,59,59,59	0
57	MG	2A	3192	1/1	0.91	0.22	66,66,66,66	0
57	MG	2A	3671	1/1	0.91	0.19	57,57,57,57	0
57	MG	1a	3253	1/1	0.91	0.13	55,55,55,55	0
57	MG	2A	3249	1/1	0.91	0.56	63,63,63,63	0
57	MG	2A	3746	1/1	0.91	0.16	49,49,49,49	0
57	MG	2A	3054	1/1	0.91	0.08	48,48,48,48	0
57	MG	1A	4061	1/1	0.91	0.13	41,41,41,41	0
57	MG	1A	3754	1/1	0.91	0.17	31,31,31,31	0
57	MG	1a	3185	1/1	0.91	0.12	54,54,54,54	0
57	MG	2A	3536	1/1	0.91	0.29	40,40,40,40	0
57	MG	1A	3514	1/1	0.91	0.21	41,41,41,41	0
57	MG	2a	3146	1/1	0.91	0.18	59,59,59,59	0
57	MG	2A	3577	1/1	0.91	0.25	63,63,63,63	0
57	MG	1A	3531	1/1	0.91	0.33	32,32,32,32	0
57	MG	1A	3768	1/1	0.91	0.07	53,53,53,53	0
57	MG	1A	3952	1/1	0.91	0.15	39,39,39,39	0
57	MG	1A	4004	1/1	0.91	0.15	38,38,38,38	0
57	MG	1A	3339	1/1	0.91	0.16	21,21,21,21	0
57	MG	2A	3416	1/1	0.91	0.21	48,48,48,48	0
57	MG	2A	3327	1/1	0.91	0.15	58,58,58,58	0
57	MG	1A	3018	1/1	0.91	0.20	26,26,26,26	0
57	MG	2a	3023	1/1	0.91	0.12	69,69,69,69	0
57	MG	1a	3189	1/1	0.91	0.19	39,39,39,39	0
57	MG	2A	3058	1/1	0.91	0.15	40,40,40,40	0
57	MG	2A	3292	1/1	0.91	0.23	38,38,38,38	0
57	MG	1A	4238	1/1	0.91	0.22	21,21,21,21	0
57	MG	2A	3324	1/1	0.91	0.20	47,47,47,47	0
57	MG	1A	3797	1/1	0.91	0.22	36,36,36,36	0
57	MG	1A	3581	1/1	0.91	0.18	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3398	1/1	0.91	0.32	39,39,39,39	0
57	MG	2a	3219	1/1	0.91	0.08	55,55,55,55	0
57	MG	1A	3309	1/1	0.91	0.27	45,45,45,45	0
57	MG	2a	3276	1/1	0.91	0.12	70,70,70,70	0
57	MG	2A	3059	1/1	0.91	0.26	49,49,49,49	0
57	MG	1A	4284	1/1	0.91	0.19	44,44,44,44	0
57	MG	2A	3667	1/1	0.91	0.15	57,57,57,57	0
57	MG	1A	3984	1/1	0.91	0.08	64,64,64,64	0
57	MG	1A	3222	1/1	0.91	0.13	31,31,31,31	0
57	MG	2A	3181	1/1	0.91	0.21	56,56,56,56	0
57	MG	1A	3580	1/1	0.91	0.10	53,53,53,53	0
57	MG	1A	3074	1/1	0.91	0.15	29,29,29,29	0
57	MG	1a	3070	1/1	0.91	0.10	46,46,46,46	0
57	MG	1A	3115	1/1	0.91	0.16	34,34,34,34	0
57	MG	1A	3791	1/1	0.91	0.13	37,37,37,37	0
57	MG	1A	4268	1/1	0.91	0.14	53,53,53,53	0
57	MG	1A	3481	1/1	0.91	0.16	45,45,45,45	0
57	MG	2A	3074	1/1	0.91	0.10	44,44,44,44	0
57	MG	1A	3880	1/1	0.91	0.16	41,41,41,41	0
57	MG	2A	3537	1/1	0.91	0.29	57,57,57,57	0
57	MG	1A	3042	1/1	0.91	0.30	48,48,48,48	0
57	MG	1A	3361	1/1	0.91	0.23	36,36,36,36	0
57	MG	1A	3310	1/1	0.91	0.20	45,45,45,45	0
57	MG	2A	3551	1/1	0.91	0.17	41,41,41,41	0
57	MG	1A	3887	1/1	0.91	0.16	35,35,35,35	0
57	MG	1A	3815	1/1	0.91	0.14	20,20,20,20	0
57	MG	1A	3017	1/1	0.91	0.47	44,44,44,44	0
57	MG	2A	3734	1/1	0.91	0.12	24,24,24,24	0
57	MG	2a	3132	1/1	0.91	0.19	49,49,49,49	0
57	MG	2A	3041	1/1	0.91	0.21	43,43,43,43	0
57	MG	2A	3441	1/1	0.91	0.14	43,43,43,43	0
57	MG	1a	3196	1/1	0.91	0.13	51,51,51,51	0
57	MG	2A	3645	1/1	0.91	0.09	40,40,40,40	0
57	MG	1A	3124	1/1	0.91	0.24	37,37,37,37	0
57	MG	1A	4143	1/1	0.91	0.14	24,24,24,24	0
57	MG	2A	3683	1/1	0.91	0.16	36,36,36,36	0
57	MG	1a	3222	1/1	0.91	0.09	35,35,35,35	0
57	MG	1A	3893	1/1	0.91	0.15	21,21,21,21	0
57	MG	1A	3359	1/1	0.91	0.22	48,48,48,48	0
57	MG	1A	3765	1/1	0.91	0.17	17,17,17,17	0
57	MG	2A	3282	1/1	0.91	0.13	47,47,47,47	0
57	MG	1A	3725	1/1	0.91	0.33	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	3569	1/1	0.91	0.26	41,41,41,41	0
57	MG	1A	3066	1/1	0.91	0.24	29,29,29,29	0
57	MG	1A	3872	1/1	0.91	0.12	58,58,58,58	0
57	MG	1A	4142	1/1	0.91	0.16	34,34,34,34	0
57	MG	1A	3856	1/1	0.91	0.12	35,35,35,35	0
57	MG	1A	3659	1/1	0.91	0.13	34,34,34,34	0
57	MG	1A	3029	1/1	0.91	0.12	51,51,51,51	0
57	MG	1A	4138	1/1	0.91	0.17	48,48,48,48	0
57	MG	1A	3691	1/1	0.91	0.18	30,30,30,30	0
57	MG	1A	3466	1/1	0.91	0.16	36,36,36,36	0
57	MG	1A	3789	1/1	0.91	0.14	49,49,49,49	0
57	MG	1A	3577	1/1	0.91	0.23	39,39,39,39	0
57	MG	1A	3777	1/1	0.91	0.18	35,35,35,35	0
57	MG	2A	3670	1/1	0.91	0.15	56,56,56,56	0
57	MG	2A	3118	1/1	0.91	0.18	54,54,54,54	0
57	MG	2A	3010	1/1	0.91	0.20	48,48,48,48	0
57	MG	2A	3651	1/1	0.91	0.13	59,59,59,59	0
57	MG	2A	3323	1/1	0.91	0.12	46,46,46,46	0
57	MG	2A	3266	1/1	0.91	0.17	47,47,47,47	0
57	MG	1A	4217	1/1	0.91	0.29	45,45,45,45	0
57	MG	1A	3634	1/1	0.91	0.11	54,54,54,54	0
57	MG	2A	3874	1/1	0.91	0.19	55,55,55,55	0
57	MG	2a	3032	1/1	0.91	0.40	74,74,74,74	0
57	MG	1A	3844	1/1	0.91	0.17	22,22,22,22	0
57	MG	2a	3088	1/1	0.91	0.12	63,63,63,63	0
57	MG	2A	3293	1/1	0.92	0.11	41,41,41,41	0
57	MG	2a	3106	1/1	0.92	0.18	56,56,56,56	0
57	MG	1A	3837	1/1	0.92	0.20	25,25,25,25	0
57	MG	1A	3098	1/1	0.92	0.19	41,41,41,41	0
57	MG	2A	3778	1/1	0.92	0.12	63,63,63,63	0
57	MG	1A	3093	1/1	0.92	0.26	42,42,42,42	0
57	MG	1A	3393	1/1	0.92	0.25	36,36,36,36	0
57	MG	1a	3114	1/1	0.92	0.12	34,34,34,34	0
57	MG	2a	3197	1/1	0.92	0.11	56,56,56,56	0
57	MG	1A	3006	1/1	0.92	0.15	47,47,47,47	0
57	MG	1A	3801	1/1	0.92	0.20	17,17,17,17	0
57	MG	2a	3166	1/1	0.92	0.17	70,70,70,70	0
57	MG	1A	3360	1/1	0.92	0.13	43,43,43,43	0
57	MG	2A	3099	1/1	0.92	0.14	55,55,55,55	0
57	MG	2A	3321	1/1	0.92	0.29	44,44,44,44	0
57	MG	1A	4266	1/1	0.92	0.11	45,45,45,45	0
57	MG	1A	3276	1/1	0.92	0.13	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3143	1/1	0.92	0.09	59,59,59,59	0
57	MG	1A	3744	1/1	0.92	0.16	32,32,32,32	0
57	MG	1A	3086	1/1	0.92	0.30	37,37,37,37	0
57	MG	1a	3054	1/1	0.92	0.19	44,44,44,44	0
57	MG	1A	3047	1/1	0.92	0.19	31,31,31,31	0
57	MG	1A	3296	1/1	0.92	0.30	29,29,29,29	0
57	MG	1A	3988	1/1	0.92	0.08	47,47,47,47	0
57	MG	1A	3432	1/1	0.92	0.11	33,33,33,33	0
57	MG	2A	3374	1/1	0.92	0.18	55,55,55,55	0
57	MG	1A	3719	1/1	0.92	0.15	36,36,36,36	0
57	MG	2a	3177	1/1	0.92	0.12	53,53,53,53	0
57	MG	2A	3934	1/1	0.92	0.18	60,60,60,60	0
57	MG	1A	4116	1/1	0.92	0.19	43,43,43,43	0
57	MG	2A	3044	1/1	0.92	0.26	53,53,53,53	0
57	MG	2A	3634	1/1	0.92	0.09	36,36,36,36	0
57	MG	2a	3051	1/1	0.92	0.18	73,73,73,73	0
57	MG	2a	3144	1/1	0.92	0.16	64,64,64,64	0
57	MG	2A	3097	1/1	0.92	0.15	40,40,40,40	0
57	MG	1A	3027	1/1	0.92	0.30	31,31,31,31	0
57	MG	1A	3619	1/1	0.92	0.17	26,26,26,26	0
57	MG	2A	3656	1/1	0.92	0.13	32,32,32,32	0
57	MG	2A	3188	1/1	0.92	0.20	42,42,42,42	0
57	MG	2A	3462	1/1	0.92	0.08	47,47,47,47	0
57	MG	2A	3392	1/1	0.92	0.09	57,57,57,57	0
57	MG	1A	3829	1/1	0.92	0.16	30,30,30,30	0
57	MG	2A	3907	1/1	0.92	0.12	34,34,34,34	0
57	MG	1A	4132	1/1	0.92	0.17	26,26,26,26	0
57	MG	2A	3871	1/1	0.92	0.18	54,54,54,54	0
57	MG	2a	3279	1/1	0.92	0.16	45,45,45,45	0
57	MG	1A	3568	1/1	0.92	0.22	41,41,41,41	0
57	MG	1A	3996	1/1	0.92	0.16	20,20,20,20	0
57	MG	1A	3218	1/1	0.92	0.12	43,43,43,43	0
57	MG	2a	3125	1/1	0.92	0.12	66,66,66,66	0
57	MG	1A	3641	1/1	0.92	0.25	31,31,31,31	0
57	MG	1A	4291	1/1	0.92	0.12	56,56,56,56	0
57	MG	1A	3287	1/1	0.92	0.19	55,55,55,55	0
57	MG	1A	4102	1/1	0.92	0.11	42,42,42,42	0
57	MG	2A	3404	1/1	0.92	0.17	45,45,45,45	0
57	MG	1A	3718	1/1	0.92	0.13	38,38,38,38	0
57	MG	2A	3430	1/1	0.92	0.27	42,42,42,42	0
57	MG	2a	3157	1/1	0.92	0.17	52,52,52,52	0
57	MG	2A	3963	1/1	0.92	0.10	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	2a	3233	1/1	0.92	0.15	67,67,67,67	0
57	MG	1A	3451	1/1	0.92	0.10	51,51,51,51	0
57	MG	1A	3020	1/1	0.92	0.41	39,39,39,39	0
57	MG	2a	3092	1/1	0.92	0.14	66,66,66,66	0
57	MG	2a	3102	1/1	0.92	0.12	48,48,48,48	0
57	MG	2A	3363	1/1	0.92	0.55	44,44,44,44	0
57	MG	1A	4289	1/1	0.92	0.11	43,43,43,43	0
57	MG	2A	3681	1/1	0.92	0.09	28,28,28,28	0
57	MG	2A	3221	1/1	0.92	0.22	50,50,50,50	0
57	MG	1A	3420	1/1	0.92	0.19	40,40,40,40	0
57	MG	1A	3494	1/1	0.92	0.19	23,23,23,23	0
57	MG	1A	3512	1/1	0.92	0.21	35,35,35,35	0
57	MG	1A	3077	1/1	0.92	0.26	62,62,62,62	0
57	MG	1A	3260	1/1	0.92	0.14	42,42,42,42	0
57	MG	2a	3123	1/1	0.92	0.18	54,54,54,54	0
57	MG	2A	3313	1/1	0.92	0.15	43,43,43,43	0
57	MG	2A	3901	1/1	0.92	0.14	50,50,50,50	0
57	MG	2A	3775	1/1	0.92	0.13	26,26,26,26	0
57	MG	1A	4194	1/1	0.92	0.07	36,36,36,36	0
57	MG	1A	3616	1/1	0.92	0.15	28,28,28,28	0
57	MG	1A	3193	1/1	0.92	0.15	33,33,33,33	0
57	MG	2A	3649	1/1	0.92	0.13	58,58,58,58	0
57	MG	2A	3183	1/1	0.92	0.12	44,44,44,44	0
57	MG	1A	3327	1/1	0.92	0.16	46,46,46,46	0
57	MG	2A	3589	1/1	0.92	0.10	42,42,42,42	0
57	MG	2A	3779	1/1	0.92	0.10	57,57,57,57	0
57	MG	2A	3463	1/1	0.92	0.31	49,49,49,49	0
57	MG	1A	4125	1/1	0.92	0.21	42,42,42,42	0
57	MG	1A	4205	1/1	0.92	0.14	41,41,41,41	0
57	MG	2A	3859	1/1	0.92	0.14	59,59,59,59	0
57	MG	2a	3081	1/1	0.92	0.28	64,64,64,64	0
57	MG	1a	3052	1/1	0.92	0.14	34,34,34,34	0
57	MG	2A	3223	1/1	0.92	0.19	36,36,36,36	0
57	MG	1A	3031	1/1	0.92	0.13	34,34,34,34	0
57	MG	1A	3758	1/1	0.92	0.11	53,53,53,53	0
57	MG	1A	3886	1/1	0.92	0.15	41,41,41,41	0
57	MG	1A	3090	1/1	0.92	0.14	23,23,23,23	0
57	MG	2A	3295	1/1	0.92	0.12	64,64,64,64	0
57	MG	2A	3277	1/1	0.92	0.23	64,64,64,64	0
57	MG	1A	3345	1/1	0.92	0.20	28,28,28,28	0
57	MG	2A	3505	1/1	0.92	0.18	50,50,50,50	0
57	MG	1A	3338	1/1	0.92	0.16	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3587	1/1	0.92	0.20	42,42,42,42	0
57	MG	1A	3079	1/1	0.92	0.18	19,19,19,19	0
57	MG	2A	3311	1/1	0.92	0.11	57,57,57,57	0
57	MG	1A	4199	1/1	0.92	0.18	37,37,37,37	0
57	MG	2A	3250	1/1	0.92	0.16	59,59,59,59	0
57	MG	1A	4007	1/1	0.92	0.14	54,54,54,54	0
57	MG	1A	3753	1/1	0.92	0.15	25,25,25,25	0
57	MG	1A	4275	1/1	0.92	0.18	40,40,40,40	0
57	MG	2A	3035	1/1	0.92	0.20	37,37,37,37	0
57	MG	1A	3426	1/1	0.92	0.19	29,29,29,29	0
57	MG	1A	3642	1/1	0.92	0.18	33,33,33,33	0
57	MG	1A	4038	1/1	0.92	0.34	50,50,50,50	0
57	MG	1A	3085	1/1	0.92	0.13	28,28,28,28	0
57	MG	2a	3066	1/1	0.92	0.19	67,67,67,67	0
57	MG	1A	3175	1/1	0.92	0.20	29,29,29,29	0
57	MG	2A	3521	1/1	0.92	0.13	51,51,51,51	0
57	MG	2a	3134	1/1	0.92	0.10	55,55,55,55	0
57	MG	1A	3448	1/1	0.92	0.25	43,43,43,43	0
57	MG	2A	3138	1/1	0.92	0.12	37,37,37,37	0
57	MG	2A	3578	1/1	0.92	0.17	52,52,52,52	0
57	MG	2A	3532	1/1	0.92	0.25	55,55,55,55	0
57	MG	1A	3939	1/1	0.92	0.20	28,28,28,28	0
57	MG	1A	3654	1/1	0.92	0.14	45,45,45,45	0
57	MG	2A	3719	1/1	0.92	0.12	38,38,38,38	0
57	MG	2A	3904	1/1	0.92	0.20	58,58,58,58	0
57	MG	1A	3080	1/1	0.92	0.19	43,43,43,43	0
57	MG	2A	3940	1/1	0.92	0.19	56,56,56,56	0
57	MG	1A	4124	1/1	0.92	0.12	33,33,33,33	0
57	MG	1A	3513	1/1	0.92	0.18	38,38,38,38	0
57	MG	1A	3968	1/1	0.92	0.21	40,40,40,40	0
57	MG	2A	3783	1/1	0.92	0.15	30,30,30,30	0
57	MG	1A	3400	1/1	0.92	0.18	45,45,45,45	0
57	MG	1A	3901	1/1	0.92	0.20	20,20,20,20	0
57	MG	1A	3724	1/1	0.92	0.43	42,42,42,42	0
57	MG	1A	3303	1/1	0.92	0.10	38,38,38,38	0
57	MG	2A	3443	1/1	0.92	0.29	41,41,41,41	0
57	MG	2A	3098	1/1	0.92	0.24	34,34,34,34	0
57	MG	1A	4054	1/1	0.92	0.28	36,36,36,36	0
57	MG	1A	3986	1/1	0.92	0.11	43,43,43,43	0
57	MG	2A	3545	1/1	0.92	0.16	29,29,29,29	0
57	MG	2A	3424	1/1	0.92	0.22	44,44,44,44	0
57	MG	1A	3475	1/1	0.92	0.21	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	1A	4254	1/1	0.92	0.24	37,37,37,37	0
57	MG	2A	3811	1/1	0.92	0.11	51,51,51,51	0
57	MG	1A	3894	1/1	0.92	0.14	23,23,23,23	0
57	MG	2A	3843	1/1	0.92	0.07	54,54,54,54	0
57	MG	1A	4055	1/1	0.92	0.16	35,35,35,35	0
57	MG	2A	3376	1/1	0.92	0.17	47,47,47,47	0
57	MG	1a	3228	1/1	0.92	0.08	56,56,56,56	0
57	MG	1A	4023	1/1	0.92	0.16	37,37,37,37	0
57	MG	1A	4264	1/1	0.92	0.14	52,52,52,52	0
57	MG	2A	3612	1/1	0.92	0.21	37,37,37,37	0
57	MG	1A	3831	1/1	0.92	0.13	22,22,22,22	0
57	MG	1a	3200	1/1	0.92	0.12	52,52,52,52	0
57	MG	2a	3155	1/1	0.92	0.24	40,40,40,40	0
57	MG	1A	3281	1/1	0.92	0.15	42,42,42,42	0
57	MG	1A	3711	1/1	0.92	0.18	33,33,33,33	0
57	MG	1A	3068	1/1	0.92	0.22	56,56,56,56	0
57	MG	2A	3092	1/1	0.92	0.14	28,28,28,28	0
57	MG	1A	3190	1/1	0.92	0.16	24,24,24,24	0
57	MG	1A	3572	1/1	0.92	0.16	38,38,38,38	0
57	MG	2A	3594	1/1	0.92	0.13	57,57,57,57	0
57	MG	1A	3406	1/1	0.92	0.15	34,34,34,34	0
57	MG	2A	3245	1/1	0.92	0.18	50,50,50,50	0
57	MG	1A	3736	1/1	0.92	0.08	52,52,52,52	0
57	MG	2A	3770	1/1	0.92	0.14	83,83,83,83	0
57	MG	1A	3643	1/1	0.92	0.25	45,45,45,45	0
57	MG	2A	3216	1/1	0.92	0.19	41,41,41,41	0
57	MG	2A	3078	1/1	0.92	0.23	38,38,38,38	0
57	MG	1a	3020	1/1	0.92	0.09	49,49,49,49	0
57	MG	1A	4177	1/1	0.92	0.08	46,46,46,46	0
57	MG	2A	3517	1/1	0.92	0.14	49,49,49,49	0
57	MG	1a	3033	1/1	0.92	0.23	47,47,47,47	0
57	MG	1A	3438	1/1	0.92	0.13	53,53,53,53	0
57	MG	1a	3160	1/1	0.92	0.20	28,28,28,28	0
57	MG	1a	3043	1/1	0.92	0.14	45,45,45,45	0
57	MG	2A	3497	1/1	0.93	0.20	48,48,48,48	0
57	MG	1A	3032	1/1	0.93	0.25	28,28,28,28	0
57	MG	1A	3464	1/1	0.93	0.20	24,24,24,24	0
57	MG	1A	3653	1/1	0.93	0.17	43,43,43,43	0
57	MG	1a	3181	1/1	0.93	0.25	61,61,61,61	0
57	MG	1a	3037	1/1	0.93	0.15	37,37,37,37	0
57	MG	2A	3706	1/1	0.93	0.12	32,32,32,32	0
57	MG	1A	3452	1/1	0.93	0.13	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	3291	1/1	0.93	0.17	38,38,38,38	0
57	MG	2A	3571	1/1	0.93	0.10	58,58,58,58	0
57	MG	1a	3064	1/1	0.93	0.10	48,48,48,48	0
57	MG	2A	3020	1/1	0.93	0.16	49,49,49,49	0
57	MG	1A	3019	1/1	0.93	0.13	36,36,36,36	0
57	MG	1a	3216	1/1	0.93	0.11	41,41,41,41	0
57	MG	2A	3889	1/1	0.93	0.11	46,46,46,46	0
57	MG	1A	3987	1/1	0.93	0.13	46,46,46,46	0
57	MG	2A	3191	1/1	0.93	0.16	43,43,43,43	0
57	MG	2A	3740	1/1	0.93	0.08	53,53,53,53	0
57	MG	1A	3835	1/1	0.93	0.12	25,25,25,25	0
57	MG	1a	3203	1/1	0.93	0.13	50,50,50,50	0
57	MG	1a	3116	1/1	0.93	0.16	43,43,43,43	0
57	MG	2a	3272	1/1	0.93	0.11	65,65,65,65	0
57	MG	1A	3955	1/1	0.93	0.17	59,59,59,59	0
57	MG	1A	3538	1/1	0.93	0.17	33,33,33,33	0
57	MG	1a	3162	1/1	0.93	0.18	51,51,51,51	0
57	MG	2A	3382	1/1	0.93	0.23	53,53,53,53	0
57	MG	1A	3441	1/1	0.93	0.15	46,46,46,46	0
57	MG	1A	3151	1/1	0.93	0.10	51,51,51,51	0
57	MG	1a	3246	1/1	0.93	0.15	49,49,49,49	0
57	MG	2a	3137	1/1	0.93	0.12	42,42,42,42	0
57	MG	2A	3655	1/1	0.93	0.15	36,36,36,36	0
57	MG	2A	3437	1/1	0.93	0.36	46,46,46,46	0
57	MG	2A	3487	1/1	0.93	0.18	54,54,54,54	0
57	MG	1A	3607	1/1	0.93	0.18	36,36,36,36	0
57	MG	2a	3274	1/1	0.93	0.16	60,60,60,60	0
57	MG	2A	3798	1/1	0.93	0.10	37,37,37,37	0
57	MG	2a	3193	1/1	0.93	0.07	74,74,74,74	0
57	MG	2A	3827	1/1	0.93	0.30	37,37,37,37	0
57	MG	1A	3270	1/1	0.93	0.29	57,57,57,57	0
57	MG	2a	3119	1/1	0.93	0.30	56,56,56,56	0
57	MG	2A	3898	1/1	0.93	0.12	28,28,28,28	0
57	MG	2A	3869	1/1	0.93	0.12	38,38,38,38	0
57	MG	1A	3752	1/1	0.93	0.18	39,39,39,39	0
57	MG	2A	3360	1/1	0.93	0.14	56,56,56,56	0
57	MG	2A	3406	1/1	0.93	0.14	48,48,48,48	0
57	MG	2A	3897	1/1	0.93	0.16	32,32,32,32	0
57	MG	2A	3630	1/1	0.93	0.21	61,61,61,61	0
57	MG	2A	3922	1/1	0.93	0.18	58,58,58,58	0
57	MG	2a	3249	1/1	0.93	0.15	62,62,62,62	0
57	MG	1A	3926	1/1	0.93	0.11	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3117	1/1	0.93	0.20	50,50,50,50	0
57	MG	2A	3547	1/1	0.93	0.27	39,39,39,39	0
57	MG	1A	3097	1/1	0.93	0.20	20,20,20,20	0
57	MG	1A	3704	1/1	0.93	0.27	44,44,44,44	0
57	MG	2A	3022	1/1	0.93	0.15	37,37,37,37	0
57	MG	2A	3347	1/1	0.93	0.11	56,56,56,56	0
57	MG	1A	4259	1/1	0.93	0.15	39,39,39,39	0
57	MG	1A	3865	1/1	0.93	0.16	54,54,54,54	0
57	MG	1A	4002	1/1	0.93	0.14	40,40,40,40	0
57	MG	1A	3743	1/1	0.93	0.21	36,36,36,36	0
57	MG	2A	3928	1/1	0.93	0.18	32,32,32,32	0
57	MG	2A	3226	1/1	0.93	0.11	43,43,43,43	0
57	MG	1A	3455	1/1	0.93	0.17	28,28,28,28	0
57	MG	1A	3727	1/1	0.93	0.10	30,30,30,30	0
57	MG	2a	3022	1/1	0.93	0.12	56,56,56,56	0
57	MG	1A	3738	1/1	0.93	0.22	40,40,40,40	0
57	MG	1A	4192	1/1	0.93	0.14	43,43,43,43	0
57	MG	2A	3119	1/1	0.93	0.23	50,50,50,50	0
57	MG	1A	3244	1/1	0.93	0.17	20,20,20,20	0
57	MG	2a	3200	1/1	0.93	0.10	78,78,78,78	0
57	MG	1A	3612	1/1	0.93	0.22	47,47,47,47	0
57	MG	2A	3495	1/1	0.93	0.26	62,62,62,62	0
57	MG	2A	3574	1/1	0.93	0.10	52,52,52,52	0
57	MG	1A	4036	1/1	0.93	0.15	28,28,28,28	0
57	MG	1A	3645	1/1	0.93	0.12	55,55,55,55	0
57	MG	2A	3385	1/1	0.93	0.13	61,61,61,61	0
57	MG	1A	3258	1/1	0.93	0.16	26,26,26,26	0
57	MG	1A	4204	1/1	0.93	0.18	43,43,43,43	0
57	MG	1A	3851	1/1	0.93	0.17	37,37,37,37	0
57	MG	2A	3553	1/1	0.93	0.23	28,28,28,28	0
57	MG	2A	3330	1/1	0.93	0.15	45,45,45,45	0
57	MG	2A	3588	1/1	0.93	0.10	62,62,62,62	0
57	MG	1A	3830	1/1	0.93	0.12	22,22,22,22	0
57	MG	1A	3823	1/1	0.93	0.09	43,43,43,43	0
57	MG	1A	3445	1/1	0.93	0.12	52,52,52,52	0
57	MG	1A	3859	1/1	0.93	0.09	36,36,36,36	0
57	MG	2A	3094	1/1	0.93	0.08	59,59,59,59	0
57	MG	1A	3465	1/1	0.93	0.14	40,40,40,40	0
57	MG	1A	3117	1/1	0.93	0.18	28,28,28,28	0
57	MG	2A	3304	1/1	0.93	0.16	42,42,42,42	0
59	ZN	2Y	501	1/1	0.93	0.12	88,88,88,88	0
57	MG	1A	3554	1/1	0.93	0.09	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	3488	1/1	0.93	0.19	38,38,38,38	0
57	MG	1A	3640	1/1	0.93	0.15	32,32,32,32	0
57	MG	2A	3708	1/1	0.93	0.23	38,38,38,38	0
57	MG	2A	3445	1/1	0.93	0.25	55,55,55,55	0
57	MG	1A	3476	1/1	0.93	0.22	28,28,28,28	0
57	MG	1A	3461	1/1	0.93	0.19	51,51,51,51	0
57	MG	1A	3947	1/1	0.93	0.12	20,20,20,20	0
57	MG	2A	3500	1/1	0.93	0.12	53,53,53,53	0
57	MG	1A	4282	1/1	0.93	0.20	27,27,27,27	0
57	MG	1A	3925	1/1	0.93	0.17	40,40,40,40	0
57	MG	1A	3354	1/1	0.93	0.16	40,40,40,40	0
57	MG	1A	3814	1/1	0.93	0.17	21,21,21,21	0
57	MG	1A	3219	1/1	0.93	0.21	19,19,19,19	0
57	MG	1A	3471	1/1	0.93	0.13	35,35,35,35	0
57	MG	2A	3830	1/1	0.93	0.17	48,48,48,48	0
57	MG	2A	3728	1/1	0.93	0.16	62,62,62,62	0
57	MG	1a	3107	1/1	0.93	0.16	46,46,46,46	0
57	MG	1a	3005	1/1	0.93	0.10	47,47,47,47	0
57	MG	1A	3661	1/1	0.93	0.25	41,41,41,41	0
57	MG	1A	4112	1/1	0.93	0.11	47,47,47,47	0
57	MG	1A	4014	1/1	0.93	0.09	29,29,29,29	0
57	MG	2A	3134	1/1	0.93	0.31	45,45,45,45	0
57	MG	1A	4106	1/1	0.93	0.11	42,42,42,42	0
57	MG	2A	3628	1/1	0.93	0.14	24,24,24,24	0
57	MG	2A	3685	1/1	0.93	0.19	39,39,39,39	0
57	MG	1A	3135	1/1	0.93	0.19	47,47,47,47	0
57	MG	1A	3256	1/1	0.93	0.15	31,31,31,31	0
57	MG	1a	3026	1/1	0.93	0.21	42,42,42,42	0
57	MG	2a	3060	1/1	0.93	0.16	62,62,62,62	0
57	MG	1A	3742	1/1	0.93	0.12	36,36,36,36	0
57	MG	2A	3419	1/1	0.93	0.25	58,58,58,58	0
57	MG	1A	3655	1/1	0.93	0.13	23,23,23,23	0
57	MG	1A	4195	1/1	0.93	0.16	17,17,17,17	0
57	MG	1A	4182	1/1	0.93	0.13	45,45,45,45	0
57	MG	2A	3417	1/1	0.93	0.11	69,69,69,69	0
57	MG	1A	3523	1/1	0.93	0.18	28,28,28,28	0
57	MG	2A	3479	1/1	0.93	0.18	57,57,57,57	0
57	MG	1A	4053	1/1	0.93	0.23	31,31,31,31	0
57	MG	1a	3123	1/1	0.93	0.25	48,48,48,48	0
57	MG	1a	3147	1/1	0.93	0.24	49,49,49,49	0
57	MG	1A	3558	1/1	0.93	0.12	66,66,66,66	0
57	MG	2A	3211	1/1	0.93	0.15	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3064	1/1	0.93	0.13	42,42,42,42	0
57	MG	2A	3236	1/1	0.93	0.22	36,36,36,36	0
57	MG	1A	4245	1/1	0.93	0.22	46,46,46,46	0
57	MG	1a	3046	1/1	0.93	0.13	41,41,41,41	0
57	MG	2A	3647	1/1	0.93	0.15	50,50,50,50	0
57	MG	1a	3242	1/1	0.93	0.18	55,55,55,55	0
57	MG	1A	3299	1/1	0.93	0.32	35,35,35,35	0
57	MG	2A	3631	1/1	0.93	0.08	42,42,42,42	0
57	MG	2A	3262	1/1	0.93	0.39	52,52,52,52	0
57	MG	2A	3351	1/1	0.93	0.10	66,66,66,66	0
57	MG	1A	3369	1/1	0.93	0.24	46,46,46,46	0
57	MG	1A	3165	1/1	0.93	0.17	32,32,32,32	0
57	MG	2A	3558	1/1	0.93	0.22	67,67,67,67	0
57	MG	2A	3540	1/1	0.93	0.20	46,46,46,46	0
57	MG	2A	3870	1/1	0.93	0.12	34,34,34,34	0
57	MG	2A	3235	1/1	0.93	0.13	57,57,57,57	0
57	MG	1A	3119	1/1	0.93	0.11	32,32,32,32	0
57	MG	1a	3057	1/1	0.93	0.16	40,40,40,40	0
57	MG	2a	3220	1/1	0.93	0.22	55,55,55,55	0
57	MG	1A	3016	1/1	0.93	0.19	43,43,43,43	0
57	MG	1A	3601	1/1	0.93	0.32	45,45,45,45	0
57	MG	2A	3458	1/1	0.93	0.21	50,50,50,50	0
57	MG	2a	3111	1/1	0.93	0.08	59,59,59,59	0
57	MG	2A	3150	1/1	0.93	0.26	42,42,42,42	0
57	MG	2A	3896	1/1	0.93	0.07	38,38,38,38	0
57	MG	1A	4091	1/1	0.93	0.13	51,51,51,51	0
57	MG	2A	3723	1/1	0.93	0.19	65,65,65,65	0
57	MG	2A	3527	1/1	0.93	0.11	57,57,57,57	0
57	MG	2A	3032	1/1	0.93	0.15	59,59,59,59	0
57	MG	2a	3029	1/1	0.93	0.12	49,49,49,49	0
57	MG	1a	3009	1/1	0.93	0.25	47,47,47,47	0
57	MG	2A	3595	1/1	0.93	0.09	41,41,41,41	0
57	MG	1a	3192	1/1	0.93	0.10	44,44,44,44	0
57	MG	2A	3937	1/1	0.93	0.11	54,54,54,54	0
57	MG	1A	3796	1/1	0.93	0.09	36,36,36,36	0
57	MG	2A	3549	1/1	0.93	0.23	33,33,33,33	0
57	MG	2A	3394	1/1	0.93	0.29	50,50,50,50	0
57	MG	1A	4241	1/1	0.93	0.15	47,47,47,47	0
57	MG	2A	3435	1/1	0.93	0.24	41,41,41,41	0
57	MG	2A	3452	1/1	0.93	0.36	53,53,53,53	0
57	MG	2A	3308	1/1	0.93	0.26	61,61,61,61	0
57	MG	2A	3219	1/1	0.93	0.10	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	3059	1/1	0.93	0.23	35,35,35,35	0
57	MG	2A	3335	1/1	0.93	0.15	38,38,38,38	0
57	MG	2a	3196	1/1	0.93	0.14	56,56,56,56	0
57	MG	1A	4235	1/1	0.93	0.18	32,32,32,32	0
57	MG	2A	3844	1/1	0.93	0.13	52,52,52,52	0
57	MG	1a	3103	1/1	0.93	0.21	56,56,56,56	0
57	MG	1A	4253	1/1	0.93	0.15	44,44,44,44	0
57	MG	2A	3436	1/1	0.93	0.22	46,46,46,46	0
57	MG	1A	3672	1/1	0.93	0.45	33,33,33,33	0
57	MG	2A	3348	1/1	0.93	0.41	44,44,44,44	0
57	MG	1a	3025	1/1	0.93	0.20	38,38,38,38	0
57	MG	1A	3078	1/1	0.93	0.10	23,23,23,23	0
57	MG	1A	4193	1/1	0.93	0.14	37,37,37,37	0
57	MG	1a	3110	1/1	0.93	0.20	39,39,39,39	0
57	MG	1A	3647	1/1	0.93	0.28	45,45,45,45	0
57	MG	2A	3255	1/1	0.93	0.16	60,60,60,60	0
57	MG	2A	3669	1/1	0.93	0.17	21,21,21,21	0
57	MG	2A	3057	1/1	0.93	0.12	60,60,60,60	0
57	MG	1A	3045	1/1	0.93	0.11	20,20,20,20	0
57	MG	2a	3087	1/1	0.93	0.15	54,54,54,54	0
57	MG	2A	3023	1/1	0.93	0.24	63,63,63,63	0
57	MG	2A	3518	1/1	0.94	0.20	46,46,46,46	0
57	MG	2A	3541	1/1	0.94	0.50	67,67,67,67	0
57	MG	2A	3912	1/1	0.94	0.09	48,48,48,48	0
57	MG	2A	3091	1/1	0.94	0.10	46,46,46,46	0
57	MG	1A	3920	1/1	0.94	0.12	31,31,31,31	0
57	MG	2A	3680	1/1	0.94	0.17	52,52,52,52	0
57	MG	1a	3133	1/1	0.94	0.11	47,47,47,47	0
57	MG	2A	3695	1/1	0.94	0.11	37,37,37,37	0
57	MG	1A	3817	1/1	0.94	0.15	22,22,22,22	0
57	MG	1A	4261	1/1	0.94	0.16	52,52,52,52	0
57	MG	1A	4224	1/1	0.94	0.11	48,48,48,48	0
57	MG	2A	3071	1/1	0.94	0.19	46,46,46,46	0
57	MG	2A	3810	1/1	0.94	0.07	50,50,50,50	0
57	MG	2A	3158	1/1	0.94	0.20	43,43,43,43	0
57	MG	1A	3820	1/1	0.94	0.10	20,20,20,20	0
57	MG	2A	3079	1/1	0.94	0.26	36,36,36,36	0
57	MG	2A	3175	1/1	0.94	0.12	56,56,56,56	0
57	MG	2A	3828	1/1	0.94	0.13	30,30,30,30	0
57	MG	1A	3041	1/1	0.94	0.29	26,26,26,26	0
57	MG	1A	3993	1/1	0.94	0.20	42,42,42,42	0
57	MG	1a	3134	1/1	0.94	0.16	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	3588	1/1	0.94	0.11	26,26,26,26	0
57	MG	1A	3565	1/1	0.94	0.21	35,35,35,35	0
57	MG	2A	3090	1/1	0.94	0.27	44,44,44,44	0
57	MG	1a	3144	1/1	0.94	0.19	46,46,46,46	0
57	MG	1A	3658	1/1	0.94	0.20	36,36,36,36	0
57	MG	2A	3519	1/1	0.94	0.14	32,32,32,32	0
57	MG	2A	3902	1/1	0.94	0.09	42,42,42,42	0
57	MG	2A	3444	1/1	0.94	0.19	41,41,41,41	0
57	MG	1A	3210	1/1	0.94	0.23	27,27,27,27	0
57	MG	1A	3595	1/1	0.94	0.21	35,35,35,35	0
57	MG	2a	3085	1/1	0.94	0.08	56,56,56,56	0
57	MG	1A	4103	1/1	0.94	0.06	24,24,24,24	0
57	MG	1a	3088	1/1	0.94	0.30	56,56,56,56	0
57	MG	1A	3548	1/1	0.94	0.23	25,25,25,25	0
57	MG	1A	3800	1/1	0.94	0.19	18,18,18,18	0
57	MG	1A	3809	1/1	0.94	0.09	32,32,32,32	0
57	MG	2A	3927	1/1	0.94	0.13	62,62,62,62	0
57	MG	2a	3245	1/1	0.94	0.09	67,67,67,67	0
57	MG	2A	3222	1/1	0.94	0.16	53,53,53,53	0
57	MG	2A	3234	1/1	0.94	0.17	51,51,51,51	0
57	MG	1a	3060	1/1	0.94	0.07	40,40,40,40	0
57	MG	2a	3259	1/1	0.94	0.06	55,55,55,55	0
57	MG	2A	3254	1/1	0.94	0.11	45,45,45,45	0
57	MG	1A	4078	1/1	0.94	0.20	28,28,28,28	0
57	MG	1A	3334	1/1	0.94	0.18	41,41,41,41	0
57	MG	2A	3012	1/1	0.94	0.09	34,34,34,34	0
57	MG	2a	3263	1/1	0.94	0.08	64,64,64,64	0
57	MG	1A	3279	1/1	0.94	0.11	34,34,34,34	0
57	MG	2A	3076	1/1	0.94	0.18	52,52,52,52	0
57	MG	2A	3280	1/1	0.94	0.10	59,59,59,59	0
57	MG	1a	3036	1/1	0.94	0.34	49,49,49,49	0
57	MG	1A	3394	1/1	0.94	0.29	42,42,42,42	0
57	MG	1A	3161	1/1	0.94	0.15	24,24,24,24	0
57	MG	2a	3124	1/1	0.94	0.07	55,55,55,55	0
57	MG	1A	4145	1/1	0.94	0.19	21,21,21,21	0
57	MG	2A	3156	1/1	0.94	0.15	60,60,60,60	0
57	MG	2A	3402	1/1	0.94	0.23	47,47,47,47	0
57	MG	1A	3930	1/1	0.94	0.17	13,13,13,13	0
57	MG	1A	3674	1/1	0.94	0.14	34,34,34,34	0
57	MG	1A	3679	1/1	0.94	0.25	42,42,42,42	0
57	MG	1A	3826	1/1	0.94	0.17	21,21,21,21	0
57	MG	1A	3770	1/1	0.94	0.16	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	3938	1/1	0.94	0.19	14,14,14,14	0
57	MG	1A	3989	1/1	0.94	0.16	46,46,46,46	0
57	MG	1A	3734	1/1	0.94	0.25	44,44,44,44	0
57	MG	2a	3039	1/1	0.94	0.13	51,51,51,51	0
57	MG	1a	3153	1/1	0.94	0.21	53,53,53,53	0
57	MG	1A	3390	1/1	0.94	0.12	49,49,49,49	0
57	MG	1A	3608	1/1	0.94	0.20	39,39,39,39	0
57	MG	1a	3223	1/1	0.94	0.12	52,52,52,52	0
57	MG	1A	4189	1/1	0.94	0.28	26,26,26,26	0
57	MG	2a	3070	1/1	0.94	0.18	46,46,46,46	0
57	MG	1A	3495	1/1	0.94	0.14	46,46,46,46	0
57	MG	2A	3489	1/1	0.94	0.11	57,57,57,57	0
57	MG	2A	3391	1/1	0.94	0.25	47,47,47,47	0
57	MG	1A	4035	1/1	0.94	0.07	27,27,27,27	0
57	MG	1A	4109	1/1	0.94	0.16	18,18,18,18	0
57	MG	1A	3428	1/1	0.94	0.12	20,20,20,20	0
57	MG	2A	3915	1/1	0.94	0.07	46,46,46,46	0
57	MG	1A	3275	1/1	0.94	0.24	36,36,36,36	0
57	MG	1A	3319	1/1	0.94	0.35	43,43,43,43	0
57	MG	1A	3171	1/1	0.94	0.22	41,41,41,41	0
57	MG	1A	3774	1/1	0.94	0.10	18,18,18,18	0
57	MG	2a	3059	1/1	0.94	0.12	50,50,50,50	0
57	MG	1A	3710	1/1	0.94	0.15	41,41,41,41	0
57	MG	1A	3793	1/1	0.94	0.17	37,37,37,37	0
57	MG	1a	3120	1/1	0.94	0.19	53,53,53,53	0
57	MG	1A	3329	1/1	0.94	0.22	41,41,41,41	0
57	MG	1A	4129	1/1	0.94	0.08	59,59,59,59	0
57	MG	2A	3075	1/1	0.94	0.14	36,36,36,36	0
57	MG	2A	3069	1/1	0.94	0.13	51,51,51,51	0
57	MG	1A	3529	1/1	0.94	0.33	38,38,38,38	0
57	MG	1A	3663	1/1	0.94	0.18	28,28,28,28	0
57	MG	2A	3003	1/1	0.94	0.28	54,54,54,54	0
57	MG	1A	3896	1/1	0.94	0.27	42,42,42,42	0
57	MG	1A	3387	1/1	0.94	0.15	35,35,35,35	0
57	MG	2A	3042	1/1	0.94	0.15	38,38,38,38	0
57	MG	1A	3050	1/1	0.94	0.13	26,26,26,26	0
57	MG	2A	3950	1/1	0.94	0.18	35,35,35,35	0
57	MG	1A	4262	1/1	0.94	0.12	20,20,20,20	0
57	MG	1A	3357	1/1	0.94	0.10	47,47,47,47	0
57	MG	1A	3998	1/1	0.94	0.19	29,29,29,29	0
57	MG	2A	3294	1/1	0.94	0.09	42,42,42,42	0
57	MG	1a	3111	1/1	0.94	0.13	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	3113	1/1	0.94	0.20	60,60,60,60	0
57	MG	1A	3539	1/1	0.94	0.18	35,35,35,35	0
57	MG	2A	3159	1/1	0.94	0.14	52,52,52,52	0
57	MG	2A	3431	1/1	0.94	0.18	35,35,35,35	0
57	MG	2a	3201	1/1	0.94	0.10	59,59,59,59	0
57	MG	2A	3720	1/1	0.94	0.10	49,49,49,49	0
57	MG	1A	3263	1/1	0.94	0.27	49,49,49,49	0
57	MG	1A	3240	1/1	0.94	0.14	35,35,35,35	0
57	MG	1A	4249	1/1	0.94	0.27	53,53,53,53	0
57	MG	1A	3380	1/1	0.94	0.22	54,54,54,54	0
57	MG	2A	3626	1/1	0.94	0.20	40,40,40,40	0
57	MG	1a	3066	1/1	0.94	0.15	51,51,51,51	0
57	MG	1A	4209	1/1	0.94	0.09	35,35,35,35	0
57	MG	2A	3763	1/1	0.94	0.20	33,33,33,33	0
57	MG	2a	3052	1/1	0.94	0.21	53,53,53,53	0
57	MG	2A	3126	1/1	0.94	0.14	48,48,48,48	0
57	MG	1A	3358	1/1	0.94	0.14	37,37,37,37	0
57	MG	2A	3932	1/1	0.94	0.27	42,42,42,42	0
57	MG	2A	3564	1/1	0.94	0.24	38,38,38,38	0
57	MG	1a	3221	1/1	0.94	0.09	46,46,46,46	0
57	MG	2A	3383	1/1	0.94	0.24	34,34,34,34	0
57	MG	2A	3713	1/1	0.94	0.12	37,37,37,37	0
57	MG	2a	3271	1/1	0.94	0.20	44,44,44,44	0
57	MG	2A	3028	1/1	0.94	0.20	38,38,38,38	0
57	MG	1A	4057	1/1	0.94	0.12	25,25,25,25	0
57	MG	1a	3146	1/1	0.94	0.18	46,46,46,46	0
57	MG	1A	3365	1/1	0.94	0.20	40,40,40,40	0
57	MG	2A	3864	1/1	0.94	0.29	64,64,64,64	0
57	MG	2a	3198	1/1	0.94	0.10	52,52,52,52	0
57	MG	1A	3586	1/1	0.94	0.15	52,52,52,52	0
57	MG	1A	3582	1/1	0.94	0.27	46,46,46,46	0
57	MG	1A	3285	1/1	0.94	0.25	35,35,35,35	0
57	MG	1A	3846	1/1	0.94	0.18	35,35,35,35	0
57	MG	1A	3288	1/1	0.94	0.26	42,42,42,42	0
57	MG	2A	3593	1/1	0.94	0.11	41,41,41,41	0
57	MG	2A	3151	1/1	0.94	0.23	52,52,52,52	0
57	MG	1A	3799	1/1	0.94	0.22	24,24,24,24	0
57	MG	1A	3212	1/1	0.94	0.21	27,27,27,27	0
57	MG	1A	3109	1/1	0.94	0.27	45,45,45,45	0
57	MG	1A	3449	1/1	0.94	0.22	41,41,41,41	0
57	MG	1A	3555	1/1	0.94	0.25	41,41,41,41	0
57	MG	2A	3855	1/1	0.94	0.17	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	3095	1/1	0.94	0.20	35,35,35,35	0
57	MG	1A	3370	1/1	0.94	0.18	22,22,22,22	0
57	MG	2A	3084	1/1	0.94	0.24	52,52,52,52	0
57	MG	2A	3858	1/1	0.94	0.08	56,56,56,56	0
57	MG	2A	3786	1/1	0.94	0.27	49,49,49,49	0
57	MG	1A	3200	1/1	0.94	0.34	38,38,38,38	0
57	MG	1A	3559	1/1	0.94	0.10	58,58,58,58	0
57	MG	1A	3351	1/1	0.94	0.20	45,45,45,45	0
57	MG	1a	3159	1/1	0.94	0.12	21,21,21,21	0
57	MG	1A	3867	1/1	0.94	0.10	56,56,56,56	0
57	MG	1A	4202	1/1	0.94	0.09	44,44,44,44	0
57	MG	1A	3533	1/1	0.94	0.12	36,36,36,36	0
57	MG	1A	4126	1/1	0.94	0.13	62,62,62,62	0
57	MG	2A	3167	1/1	0.94	0.19	47,47,47,47	0
57	MG	2A	3709	1/1	0.94	0.15	60,60,60,60	0
57	MG	2A	3566	1/1	0.94	0.29	43,43,43,43	0
57	MG	2A	3171	1/1	0.94	0.22	47,47,47,47	0
57	MG	2a	3202	1/1	0.94	0.15	62,62,62,62	0
57	MG	1A	3490	1/1	0.94	0.51	34,34,34,34	0
57	MG	1A	4207	1/1	0.94	0.11	16,16,16,16	0
57	MG	1A	4260	1/1	0.94	0.23	45,45,45,45	0
57	MG	1A	3683	1/1	0.94	0.22	42,42,42,42	0
57	MG	1A	3107	1/1	0.94	0.14	26,26,26,26	0
57	MG	2a	3065	1/1	0.94	0.08	55,55,55,55	0
57	MG	1A	3798	1/1	0.94	0.16	30,30,30,30	0
57	MG	1A	3063	1/1	0.94	0.11	23,23,23,23	0
57	MG	2A	3768	1/1	0.94	0.21	57,57,57,57	0
57	MG	1A	3847	1/1	0.94	0.18	24,24,24,24	0
57	MG	1a	3240	1/1	0.94	0.11	55,55,55,55	0
57	MG	2a	3218	1/1	0.94	0.30	58,58,58,58	0
59	ZN	24	501	1/1	0.94	0.13	114,114,114,114	0
57	MG	1A	3589	1/1	0.94	0.15	29,29,29,29	0
57	MG	1A	3717	1/1	0.94	0.14	28,28,28,28	0
57	MG	1A	3242	1/1	0.94	0.12	33,33,33,33	0
57	MG	1A	4298	1/1	0.94	0.11	52,52,52,52	0
57	MG	1A	3772	1/1	0.94	0.19	46,46,46,46	0
57	MG	2A	3806	1/1	0.94	0.14	42,42,42,42	0
57	MG	2a	3096	1/1	0.94	0.14	48,48,48,48	0
57	MG	1A	4045	1/1	0.94	0.14	44,44,44,44	0
57	MG	1A	3638	1/1	0.94	0.18	25,25,25,25	0
57	MG	1a	3019	1/1	0.94	0.12	46,46,46,46	0
57	MG	1A	4118	1/1	0.94	0.08	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3067	1/1	0.94	0.11	56,56,56,56	0
57	MG	2A	3507	1/1	0.94	0.19	33,33,33,33	0
57	MG	2A	3743	1/1	0.94	0.12	52,52,52,52	0
57	MG	1a	3099	1/1	0.94	0.20	45,45,45,45	0
57	MG	1A	4107	1/1	0.94	0.07	45,45,45,45	0
57	MG	2a	3171	1/1	0.94	0.31	46,46,46,46	0
57	MG	1A	4137	1/1	0.94	0.45	37,37,37,37	0
57	MG	2A	3247	1/1	0.94	0.18	49,49,49,49	0
57	MG	2A	3269	1/1	0.94	0.12	45,45,45,45	0
57	MG	1A	3693	1/1	0.94	0.17	34,34,34,34	0
57	MG	2A	3542	1/1	0.94	0.32	53,53,53,53	0
57	MG	1a	3129	1/1	0.94	0.26	32,32,32,32	0
57	MG	1A	3278	1/1	0.94	0.18	32,32,32,32	0
57	MG	1A	4048	1/1	0.94	0.21	24,24,24,24	0
57	MG	1A	3576	1/1	0.94	0.26	21,21,21,21	0
57	MG	1A	3511	1/1	0.94	0.22	29,29,29,29	0
57	MG	1a	3047	1/1	0.94	0.17	42,42,42,42	0
57	MG	1A	3803	1/1	0.94	0.15	28,28,28,28	0
57	MG	2A	3388	1/1	0.94	0.23	63,63,63,63	0
57	MG	1a	3077	1/1	0.94	0.10	40,40,40,40	0
57	MG	2A	3372	1/1	0.94	0.12	49,49,49,49	0
57	MG	2a	3053	1/1	0.94	0.31	60,60,60,60	0
57	MG	1A	4071	1/1	0.94	0.13	46,46,46,46	0
57	MG	2A	3957	1/1	0.94	0.18	42,42,42,42	0
57	MG	1a	3048	1/1	0.94	0.09	51,51,51,51	0
57	MG	1A	3147	1/1	0.94	0.17	35,35,35,35	0
57	MG	2A	3165	1/1	0.94	0.20	59,59,59,59	0
57	MG	1A	3882	1/1	0.94	0.22	28,28,28,28	0
57	MG	2A	3916	1/1	0.94	0.19	18,18,18,18	0
57	MG	2a	3205	1/1	0.94	0.13	42,42,42,42	0
57	MG	1A	3008	1/1	0.94	0.16	24,24,24,24	0
57	MG	1A	3714	1/1	0.94	0.15	37,37,37,37	0
57	MG	2a	3150	1/1	0.94	0.21	39,39,39,39	0
57	MG	2A	3959	1/1	0.94	0.18	49,49,49,49	0
57	MG	1A	3082	1/1	0.94	0.16	23,23,23,23	0
57	MG	1A	3246	1/1	0.94	0.22	31,31,31,31	0
57	MG	1A	4257	1/1	0.94	0.12	60,60,60,60	0
57	MG	1a	3184	1/1	0.94	0.14	39,39,39,39	0
57	MG	1A	3840	1/1	0.94	0.20	23,23,23,23	0
57	MG	2A	3894	1/1	0.94	0.12	29,29,29,29	0
57	MG	2A	3891	1/1	0.94	0.16	31,31,31,31	0
57	MG	1A	3430	1/1	0.94	0.22	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	1A	4162	1/1	0.94	0.15	44,44,44,44	0
57	MG	2A	3580	1/1	0.94	0.21	53,53,53,53	0
57	MG	1A	3022	1/1	0.94	0.12	40,40,40,40	0
57	MG	1A	3087	1/1	0.94	0.23	38,38,38,38	0
57	MG	2A	3793	1/1	0.94	0.09	50,50,50,50	0
57	MG	2a	3195	1/1	0.94	0.18	57,57,57,57	0
57	MG	1A	3434	1/1	0.94	0.34	46,46,46,46	0
57	MG	1A	3889	1/1	0.94	0.12	36,36,36,36	0
57	MG	1A	3700	1/1	0.94	0.20	35,35,35,35	0
57	MG	2A	3169	1/1	0.95	0.24	32,32,32,32	0
57	MG	2a	3230	1/1	0.95	0.19	49,49,49,49	0
57	MG	2a	3098	1/1	0.95	0.08	67,67,67,67	0
57	MG	1a	3058	1/1	0.95	0.24	49,49,49,49	0
57	MG	2a	3142	1/1	0.95	0.23	59,59,59,59	0
57	MG	1A	4089	1/1	0.95	0.12	43,43,43,43	0
57	MG	1A	3409	1/1	0.95	0.26	24,24,24,24	0
57	MG	1A	3142	1/1	0.95	0.12	28,28,28,28	0
57	MG	2A	3674	1/1	0.95	0.21	56,56,56,56	0
57	MG	1A	3516	1/1	0.95	0.28	40,40,40,40	0
57	MG	1A	4206	1/1	0.95	0.10	23,23,23,23	0
57	MG	2A	3794	1/1	0.95	0.16	57,57,57,57	0
57	MG	1A	4287	1/1	0.95	0.21	35,35,35,35	0
57	MG	1A	3934	1/1	0.95	0.15	29,29,29,29	0
57	MG	2A	3352	1/1	0.95	0.14	45,45,45,45	0
57	MG	1A	3433	1/1	0.95	0.10	36,36,36,36	0
57	MG	2A	3112	1/1	0.95	0.22	36,36,36,36	0
57	MG	1A	3130	1/1	0.95	0.15	24,24,24,24	0
57	MG	1A	3579	1/1	0.95	0.25	53,53,53,53	0
57	MG	2A	3231	1/1	0.95	0.26	51,51,51,51	0
57	MG	1A	3245	1/1	0.95	0.20	25,25,25,25	0
57	MG	1A	3722	1/1	0.95	0.21	29,29,29,29	0
57	MG	1A	3458	1/1	0.95	0.19	38,38,38,38	0
57	MG	1A	4115	1/1	0.95	0.16	43,43,43,43	0
57	MG	2a	3013	1/1	0.95	0.14	40,40,40,40	0
57	MG	1A	3973	1/1	0.95	0.18	47,47,47,47	0
57	MG	1A	4221	1/1	0.95	0.25	41,41,41,41	0
57	MG	2A	3767	1/1	0.95	0.16	43,43,43,43	0
57	MG	2A	3370	1/1	0.95	0.13	52,52,52,52	0
57	MG	1a	3238	1/1	0.95	0.17	64,64,64,64	0
57	MG	2A	3677	1/1	0.95	0.16	36,36,36,36	0
57	MG	2A	3839	1/1	0.95	0.16	34,34,34,34	0
57	MG	1A	3964	1/1	0.95	0.17	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1a	3079	1/1	0.95	0.17	40,40,40,40	0
57	MG	1A	3759	1/1	0.95	0.19	18,18,18,18	0
57	MG	1A	3129	1/1	0.95	0.16	42,42,42,42	0
57	MG	1a	3071	1/1	0.95	0.15	51,51,51,51	0
57	MG	2A	3662	1/1	0.95	0.18	28,28,28,28	0
57	MG	2a	3187	1/1	0.95	0.14	62,62,62,62	0
57	MG	1a	3186	1/1	0.95	0.20	46,46,46,46	0
57	MG	1A	3136	1/1	0.95	0.22	22,22,22,22	0
57	MG	2a	3210	1/1	0.95	0.09	49,49,49,49	0
57	MG	1A	3562	1/1	0.95	0.14	35,35,35,35	0
57	MG	2A	3572	1/1	0.95	0.13	46,46,46,46	0
57	MG	1A	3292	1/1	0.95	0.18	28,28,28,28	0
57	MG	1A	4234	1/1	0.95	0.14	38,38,38,38	0
57	MG	2A	3464	1/1	0.95	0.24	59,59,59,59	0
57	MG	1A	3305	1/1	0.95	0.14	27,27,27,27	0
57	MG	1A	3757	1/1	0.95	0.25	25,25,25,25	0
57	MG	1A	3277	1/1	0.95	0.12	32,32,32,32	0
57	MG	2A	3110	1/1	0.95	0.25	44,44,44,44	0
57	MG	1A	3850	1/1	0.95	0.25	43,43,43,43	0
57	MG	1A	3566	1/1	0.95	0.17	35,35,35,35	0
57	MG	1A	3524	1/1	0.95	0.21	37,37,37,37	0
57	MG	2A	3817	1/1	0.95	0.13	49,49,49,49	0
57	MG	2a	3100	1/1	0.95	0.24	44,44,44,44	0
57	MG	1A	3992	1/1	0.95	0.21	14,14,14,14	0
57	MG	1A	4272	1/1	0.95	0.11	41,41,41,41	0
57	MG	2a	3189	1/1	0.95	0.07	61,61,61,61	0
57	MG	1A	3149	1/1	0.95	0.23	16,16,16,16	0
57	MG	2A	3051	1/1	0.95	0.18	25,25,25,25	0
57	MG	1A	3863	1/1	0.95	0.19	35,35,35,35	0
57	MG	2a	3231	1/1	0.95	0.11	69,69,69,69	0
57	MG	1A	4050	1/1	0.95	0.12	30,30,30,30	0
57	MG	2a	3026	1/1	0.95	0.97	68,68,68,68	0
57	MG	2A	3371	1/1	0.95	0.08	49,49,49,49	0
57	MG	1A	4176	1/1	0.95	0.15	24,24,24,24	0
57	MG	1A	3172	1/1	0.95	0.13	51,51,51,51	0
57	MG	2A	3569	1/1	0.95	0.12	57,57,57,57	0
57	MG	2A	3206	1/1	0.95	0.12	51,51,51,51	0
57	MG	1A	4265	1/1	0.95	0.13	44,44,44,44	0
57	MG	1A	4121	1/1	0.95	0.12	26,26,26,26	0
57	MG	1A	3344	1/1	0.95	0.27	42,42,42,42	0
57	MG	2a	3206	1/1	0.95	0.14	60,60,60,60	0
57	MG	1A	3199	1/1	0.95	0.12	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	4219	1/1	0.95	0.17	47,47,47,47	0
57	MG	1A	3644	1/1	0.95	0.09	56,56,56,56	0
57	MG	2A	3801	1/1	0.95	0.19	44,44,44,44	0
57	MG	1A	3932	1/1	0.95	0.21	48,48,48,48	0
57	MG	2A	3646	1/1	0.95	0.18	23,23,23,23	0
57	MG	2A	3320	1/1	0.95	0.08	61,61,61,61	0
57	MG	2A	3471	1/1	0.95	0.28	36,36,36,36	0
57	MG	1A	3108	1/1	0.95	0.18	28,28,28,28	0
57	MG	1A	3598	1/1	0.95	0.26	29,29,29,29	0
57	MG	1A	3325	1/1	0.95	0.33	46,46,46,46	0
57	MG	1a	3101	1/1	0.95	0.28	42,42,42,42	0
57	MG	1A	3692	1/1	0.95	0.22	27,27,27,27	0
57	MG	1A	3696	1/1	0.95	0.11	55,55,55,55	0
57	MG	2A	3845	1/1	0.95	0.13	52,52,52,52	0
57	MG	1A	3081	1/1	0.95	0.11	24,24,24,24	0
57	MG	2a	3099	1/1	0.95	0.19	42,42,42,42	0
57	MG	2A	3440	1/1	0.95	0.16	30,30,30,30	0
57	MG	1a	3124	1/1	0.95	0.27	41,41,41,41	0
57	MG	2A	3102	1/1	0.95	0.18	40,40,40,40	0
57	MG	2A	3180	1/1	0.95	0.17	44,44,44,44	0
57	MG	2A	3147	1/1	0.95	0.20	27,27,27,27	0
57	MG	2A	3309	1/1	0.95	0.38	60,60,60,60	0
57	MG	1A	3482	1/1	0.95	0.23	33,33,33,33	0
57	MG	1A	4173	1/1	0.95	0.13	42,42,42,42	0
57	MG	2A	3393	1/1	0.95	0.21	30,30,30,30	0
57	MG	2A	3017	1/1	0.95	0.13	40,40,40,40	0
57	MG	2A	3346	1/1	0.95	0.22	53,53,53,53	0
57	MG	1A	4161	1/1	0.95	0.17	42,42,42,42	0
57	MG	1A	3802	1/1	0.95	0.12	41,41,41,41	0
57	MG	1a	3137	1/1	0.95	0.19	64,64,64,64	0
57	MG	1A	4256	1/1	0.95	0.23	34,34,34,34	0
57	MG	1A	4034	1/1	0.95	0.10	33,33,33,33	0
57	MG	2A	3781	1/1	0.95	0.13	30,30,30,30	0
57	MG	2a	3252	1/1	0.95	0.26	61,61,61,61	0
57	MG	1A	3366	1/1	0.95	0.14	28,28,28,28	0
57	MG	2A	3526	1/1	0.95	0.19	54,54,54,54	0
57	MG	1A	3183	1/1	0.95	0.39	30,30,30,30	0
57	MG	1A	3750	1/1	0.95	0.16	38,38,38,38	0
57	MG	2A	3528	1/1	0.95	0.17	30,30,30,30	0
57	MG	2A	3682	1/1	0.95	0.17	23,23,23,23	0
57	MG	1A	3103	1/1	0.95	0.16	32,32,32,32	0
57	MG	1A	3963	1/1	0.95	0.13	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	2A	3900	1/1	0.95	0.09	35,35,35,35	0
57	MG	1A	4037	1/1	0.95	0.19	16,16,16,16	0
57	MG	2a	3257	1/1	0.95	0.11	44,44,44,44	0
57	MG	1A	4215	1/1	0.95	0.17	38,38,38,38	0
57	MG	1A	3265	1/1	0.95	0.20	20,20,20,20	0
57	MG	1A	3561	1/1	0.95	0.15	51,51,51,51	0
57	MG	1A	3100	1/1	0.95	0.29	31,31,31,31	0
57	MG	2a	3025	1/1	0.95	0.11	50,50,50,50	0
57	MG	2A	3339	1/1	0.95	0.37	46,46,46,46	0
57	MG	2A	3189	1/1	0.95	0.14	32,32,32,32	0
57	MG	2A	3080	1/1	0.95	0.16	39,39,39,39	0
57	MG	2a	3138	1/1	0.95	0.16	59,59,59,59	0
57	MG	1A	3545	1/1	0.95	0.16	46,46,46,46	0
57	MG	1A	3225	1/1	0.95	0.25	30,30,30,30	0
57	MG	2A	3809	1/1	0.95	0.09	44,44,44,44	0
57	MG	2A	3597	1/1	0.95	0.08	31,31,31,31	0
57	MG	2A	3114	1/1	0.95	0.13	48,48,48,48	0
57	MG	2A	3123	1/1	0.95	0.19	37,37,37,37	0
57	MG	1a	3035	1/1	0.95	0.14	54,54,54,54	0
57	MG	1A	4094	1/1	0.95	0.08	46,46,46,46	0
57	MG	1A	3885	1/1	0.95	0.25	48,48,48,48	0
57	MG	2A	3038	1/1	0.95	0.07	52,52,52,52	0
57	MG	2A	3506	1/1	0.95	0.15	49,49,49,49	0
57	MG	1a	3085	1/1	0.95	0.14	54,54,54,54	0
57	MG	2A	3754	1/1	0.95	0.22	46,46,46,46	0
57	MG	1A	3233	1/1	0.95	0.24	50,50,50,50	0
57	MG	1A	4101	1/1	0.95	0.12	30,30,30,30	0
57	MG	1A	3575	1/1	0.95	0.17	54,54,54,54	0
57	MG	1A	3587	1/1	0.95	0.07	42,42,42,42	0
57	MG	1A	3375	1/1	0.95	0.21	34,34,34,34	0
57	MG	2a	3176	1/1	0.95	0.29	46,46,46,46	0
57	MG	1A	3979	1/1	0.95	0.10	48,48,48,48	0
57	MG	1A	3196	1/1	0.95	0.24	34,34,34,34	0
57	MG	1A	3053	1/1	0.95	0.20	23,23,23,23	0
57	MG	1a	3078	1/1	0.95	0.11	47,47,47,47	0
57	MG	1A	4096	1/1	0.95	0.24	48,48,48,48	0
57	MG	1A	4277	1/1	0.95	0.13	40,40,40,40	0
57	MG	1A	4030	1/1	0.95	0.18	35,35,35,35	0
57	MG	2A	3879	1/1	0.95	0.17	52,52,52,52	0
57	MG	2A	3962	1/1	0.95	0.13	47,47,47,47	0
57	MG	2A	3729	1/1	0.95	0.08	60,60,60,60	0
57	MG	1A	3454	1/1	0.95	0.17	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3461	1/1	0.95	0.24	37,37,37,37	0
57	MG	2A	3846	1/1	0.95	0.10	44,44,44,44	0
57	MG	1a	3177	1/1	0.95	0.10	34,34,34,34	0
57	MG	1A	3477	1/1	0.95	0.16	31,31,31,31	0
57	MG	1A	3266	1/1	0.95	0.13	51,51,51,51	0
57	MG	1A	4233	1/1	0.95	0.14	61,61,61,61	0
57	MG	1A	3552	1/1	0.95	0.24	23,23,23,23	0
57	MG	2A	3432	1/1	0.95	0.28	40,40,40,40	0
57	MG	1A	3111	1/1	0.95	0.16	21,21,21,21	0
57	MG	1A	4214	1/1	0.95	0.14	44,44,44,44	0
57	MG	2A	3946	1/1	0.95	0.26	47,47,47,47	0
57	MG	1A	4031	1/1	0.95	0.15	46,46,46,46	0
57	MG	1A	3767	1/1	0.95	0.07	32,32,32,32	0
57	MG	2A	3818	1/1	0.95	0.20	38,38,38,38	0
57	MG	1A	3870	1/1	0.95	0.12	20,20,20,20	0
57	MG	1A	3217	1/1	0.95	0.16	31,31,31,31	0
57	MG	2A	3848	1/1	0.95	0.14	46,46,46,46	0
57	MG	1a	3093	1/1	0.95	0.22	46,46,46,46	0
57	MG	1A	3389	1/1	0.95	0.30	54,54,54,54	0
57	MG	2a	3178	1/1	0.95	0.20	43,43,43,43	0
57	MG	1A	3379	1/1	0.95	0.29	45,45,45,45	0
57	MG	1A	3918	1/1	0.95	0.13	20,20,20,20	0
57	MG	1A	3060	1/1	0.95	0.22	30,30,30,30	0
57	MG	1A	3184	1/1	0.95	0.16	33,33,33,33	0
57	MG	2A	3007	1/1	0.95	0.19	45,45,45,45	0
57	MG	1a	3044	1/1	0.95	0.11	41,41,41,41	0
57	MG	1A	4041	1/1	0.95	0.16	32,32,32,32	0
57	MG	2A	3420	1/1	0.95	0.24	42,42,42,42	0
57	MG	2A	3081	1/1	0.95	0.16	18,18,18,18	0
57	MG	2A	3390	1/1	0.95	0.15	45,45,45,45	0
57	MG	2A	3952	1/1	0.95	0.13	65,65,65,65	0
57	MG	2A	3652	1/1	0.95	0.16	48,48,48,48	0
57	MG	1A	3297	1/1	0.95	0.24	24,24,24,24	0
57	MG	1A	4076	1/1	0.95	0.14	26,26,26,26	0
57	MG	2A	3745	1/1	0.95	0.11	54,54,54,54	0
57	MG	1A	3536	1/1	0.95	0.15	49,49,49,49	0
57	MG	2A	3688	1/1	0.95	0.15	44,44,44,44	0
57	MG	1A	4178	1/1	0.95	0.13	43,43,43,43	0
57	MG	1A	3498	1/1	0.95	0.25	45,45,45,45	0
57	MG	1A	3280	1/1	0.95	0.12	41,41,41,41	0
57	MG	1A	3286	1/1	0.95	0.19	37,37,37,37	0
57	MG	1A	3713	1/1	0.95	0.25	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	3116	1/1	0.95	0.10	19,19,19,19	0
57	MG	2A	3772	1/1	0.95	0.09	55,55,55,55	0
57	MG	1A	4020	1/1	0.95	0.12	27,27,27,27	0
57	MG	1A	3549	1/1	0.95	0.15	24,24,24,24	0
57	MG	2A	3954	1/1	0.95	0.11	49,49,49,49	0
57	MG	1A	3155	1/1	0.95	0.17	31,31,31,31	0
57	MG	1A	3049	1/1	0.95	0.14	23,23,23,23	0
57	MG	1A	4220	1/1	0.95	0.23	39,39,39,39	0
57	MG	1A	3463	1/1	0.95	0.12	41,41,41,41	0
57	MG	1a	3239	1/1	0.95	0.26	41,41,41,41	0
57	MG	2a	3089	1/1	0.95	0.10	52,52,52,52	0
57	MG	1A	3126	1/1	0.95	0.15	31,31,31,31	0
57	MG	1A	3650	1/1	0.95	0.22	43,43,43,43	0
57	MG	1A	3105	1/1	0.95	0.18	38,38,38,38	0
57	MG	1A	4099	1/1	0.95	0.13	48,48,48,48	0
57	MG	2a	3194	1/1	0.95	0.13	50,50,50,50	0
57	MG	2A	3125	1/1	0.95	0.05	67,67,67,67	0
57	MG	1A	3489	1/1	0.95	0.24	39,39,39,39	0
57	MG	1A	3340	1/1	0.95	0.14	46,46,46,46	0
57	MG	2A	3550	1/1	0.95	0.21	45,45,45,45	0
57	MG	1A	3304	1/1	0.95	0.20	40,40,40,40	0
57	MG	1A	3909	1/1	0.95	0.14	25,25,25,25	0
57	MG	1A	3869	1/1	0.95	0.14	33,33,33,33	0
57	MG	1A	3001	1/1	0.95	0.15	31,31,31,31	0
57	MG	1A	3203	1/1	0.95	0.14	27,27,27,27	0
57	MG	1A	3118	1/1	0.95	0.22	23,23,23,23	0
57	MG	1a	3118	1/1	0.95	0.27	44,44,44,44	0
57	MG	1A	3689	1/1	0.95	0.16	34,34,34,34	0
57	MG	2A	3707	1/1	0.95	0.11	39,39,39,39	0
57	MG	2A	3617	1/1	0.95	0.12	42,42,42,42	0
57	MG	2A	3766	1/1	0.96	0.24	46,46,46,46	0
57	MG	2A	3586	1/1	0.96	0.13	50,50,50,50	0
57	MG	1A	3088	1/1	0.96	0.22	29,29,29,29	0
57	MG	1A	3787	1/1	0.96	0.12	29,29,29,29	0
57	MG	1A	3976	1/1	0.96	0.10	25,25,25,25	0
57	MG	2A	3807	1/1	0.96	0.19	39,39,39,39	0
57	MG	1A	3174	1/1	0.96	0.29	28,28,28,28	0
57	MG	1A	4196	1/1	0.96	0.11	42,42,42,42	0
57	MG	2A	3939	1/1	0.96	0.22	30,30,30,30	0
57	MG	1A	3697	1/1	0.96	0.23	37,37,37,37	0
57	MG	2A	3157	1/1	0.96	0.28	51,51,51,51	0
57	MG	1A	3816	1/1	0.96	0.20	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	3123	1/1	0.96	0.20	26,26,26,26	0
57	MG	2A	3350	1/1	0.96	0.08	58,58,58,58	0
57	MG	1A	4150	1/1	0.96	0.09	77,77,77,77	0
57	MG	2A	3796	1/1	0.96	0.14	38,38,38,38	0
57	MG	2A	3849	1/1	0.96	0.14	31,31,31,31	0
57	MG	1A	3141	1/1	0.96	0.37	34,34,34,34	0
57	MG	2A	3725	1/1	0.96	0.13	41,41,41,41	0
57	MG	1A	3902	1/1	0.96	0.13	27,27,27,27	0
57	MG	1A	3923	1/1	0.96	0.17	17,17,17,17	0
57	MG	1A	3322	1/1	0.96	0.14	28,28,28,28	0
57	MG	2A	3620	1/1	0.96	0.11	27,27,27,27	0
57	MG	2a	3212	1/1	0.96	0.12	38,38,38,38	0
57	MG	2A	3490	1/1	0.96	0.19	59,59,59,59	0
57	MG	1A	3745	1/1	0.96	0.13	37,37,37,37	0
57	MG	1A	3746	1/1	0.96	0.17	23,23,23,23	0
57	MG	2a	3006	1/1	0.96	0.19	49,49,49,49	0
57	MG	2A	3544	1/1	0.96	0.16	19,19,19,19	0
57	MG	2A	3654	1/1	0.96	0.13	42,42,42,42	0
57	MG	1A	3274	1/1	0.96	0.12	53,53,53,53	0
57	MG	2A	3769	1/1	0.96	0.15	56,56,56,56	0
57	MG	1A	4062	1/1	0.96	0.10	23,23,23,23	0
57	MG	1A	3249	1/1	0.96	0.15	44,44,44,44	0
57	MG	2a	3224	1/1	0.96	0.12	47,47,47,47	0
57	MG	1A	3981	1/1	0.96	0.15	29,29,29,29	0
57	MG	1A	3864	1/1	0.96	0.07	60,60,60,60	0
57	MG	2A	3945	1/1	0.96	0.13	42,42,42,42	0
57	MG	1A	3748	1/1	0.96	0.16	24,24,24,24	0
57	MG	1a	3014	1/1	0.96	0.24	52,52,52,52	0
57	MG	1A	3341	1/1	0.96	0.12	35,35,35,35	0
57	MG	2A	3055	1/1	0.96	0.16	64,64,64,64	0
57	MG	2A	3618	1/1	0.96	0.11	37,37,37,37	0
57	MG	1A	3496	1/1	0.96	0.16	27,27,27,27	0
57	MG	2a	3104	1/1	0.96	0.17	41,41,41,41	0
57	MG	1a	3213	1/1	0.96	0.05	40,40,40,40	0
57	MG	1A	3834	1/1	0.96	0.15	35,35,35,35	0
57	MG	2a	3258	1/1	0.96	0.11	49,49,49,49	0
57	MG	1A	3048	1/1	0.96	0.18	17,17,17,17	0
57	MG	1A	4213	1/1	0.96	0.13	42,42,42,42	0
57	MG	2A	3602	1/1	0.96	0.11	39,39,39,39	0
57	MG	1A	4288	1/1	0.96	0.09	49,49,49,49	0
57	MG	1A	3069	1/1	0.96	0.16	27,27,27,27	0
57	MG	1A	4281	1/1	0.96	0.17	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	3218	1/1	0.96	0.09	53,53,53,53	0
57	MG	2A	3635	1/1	0.96	0.07	40,40,40,40	0
57	MG	2A	3570	1/1	0.96	0.18	41,41,41,41	0
57	MG	2a	3246	1/1	0.96	0.09	48,48,48,48	0
57	MG	1A	3442	1/1	0.96	0.13	34,34,34,34	0
57	MG	1A	3701	1/1	0.96	0.18	39,39,39,39	0
57	MG	1A	4148	1/1	0.96	0.07	42,42,42,42	0
57	MG	1A	3073	1/1	0.96	0.19	16,16,16,16	0
57	MG	1A	3764	1/1	0.96	0.10	50,50,50,50	0
57	MG	1a	3090	1/1	0.96	0.22	31,31,31,31	0
57	MG	2A	3600	1/1	0.96	0.17	29,29,29,29	0
57	MG	2A	3861	1/1	0.96	0.08	56,56,56,56	0
57	MG	1A	3101	1/1	0.96	0.15	26,26,26,26	0
57	MG	2A	3856	1/1	0.96	0.09	64,64,64,64	0
57	MG	1A	3474	1/1	0.96	0.20	28,28,28,28	0
57	MG	2A	3002	1/1	0.96	0.24	46,46,46,46	0
57	MG	2A	3063	1/1	0.96	0.11	42,42,42,42	0
57	MG	1A	4039	1/1	0.96	0.13	34,34,34,34	0
57	MG	1A	3888	1/1	0.96	0.29	37,37,37,37	0
57	MG	1A	3649	1/1	0.96	0.12	36,36,36,36	0
57	MG	1A	3023	1/1	0.96	0.17	11,11,11,11	0
57	MG	1A	4190	1/1	0.96	0.18	20,20,20,20	0
57	MG	2A	3423	1/1	0.96	0.15	51,51,51,51	0
57	MG	2A	3774	1/1	0.96	0.14	55,55,55,55	0
57	MG	1A	3526	1/1	0.96	0.32	50,50,50,50	0
57	MG	1A	3720	1/1	0.96	0.14	25,25,25,25	0
57	MG	2A	3013	1/1	0.96	0.15	35,35,35,35	0
57	MG	1a	3142	1/1	0.96	0.21	54,54,54,54	0
57	MG	1A	3180	1/1	0.96	0.30	36,36,36,36	0
57	MG	1A	3321	1/1	0.96	0.26	23,23,23,23	0
57	MG	1A	4113	1/1	0.96	0.16	47,47,47,47	0
57	MG	1a	3154	1/1	0.96	0.12	61,61,61,61	0
57	MG	2A	3449	1/1	0.96	0.28	38,38,38,38	0
57	MG	2A	3009	1/1	0.96	0.13	36,36,36,36	0
57	MG	2A	3737	1/1	0.96	0.24	63,63,63,63	0
57	MG	1A	3160	1/1	0.96	0.23	29,29,29,29	0
57	MG	1A	3343	1/1	0.96	0.23	36,36,36,36	0
57	MG	1A	3473	1/1	0.96	0.22	37,37,37,37	0
57	MG	1A	3942	1/1	0.96	0.12	29,29,29,29	0
57	MG	2A	3130	1/1	0.96	0.16	45,45,45,45	0
57	MG	1A	4021	1/1	0.96	0.25	34,34,34,34	0
57	MG	2A	3877	1/1	0.96	0.07	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	2A	3064	1/1	0.96	0.13	40,40,40,40	0
57	MG	1A	3806	1/1	0.96	0.13	24,24,24,24	0
57	MG	1A	4191	1/1	0.96	0.14	27,27,27,27	0
57	MG	2A	3395	1/1	0.96	0.13	39,39,39,39	0
57	MG	1A	3021	1/1	0.96	0.13	19,19,19,19	0
57	MG	2A	3814	1/1	0.96	0.15	47,47,47,47	0
57	MG	2A	3207	1/1	0.96	0.14	43,43,43,43	0
57	MG	1A	3705	1/1	0.96	0.36	32,32,32,32	0
57	MG	2a	3112	1/1	0.96	0.19	54,54,54,54	0
57	MG	1A	3122	1/1	0.96	0.19	22,22,22,22	0
57	MG	1A	3967	1/1	0.96	0.13	35,35,35,35	0
57	MG	2A	3668	1/1	0.96	0.24	63,63,63,63	0
57	MG	1A	3055	1/1	0.96	0.09	24,24,24,24	0
57	MG	1A	4185	1/1	0.96	0.29	46,46,46,46	0
57	MG	1A	3790	1/1	0.96	0.10	28,28,28,28	0
57	MG	1A	3741	1/1	0.96	0.14	24,24,24,24	0
57	MG	1a	3241	1/1	0.96	0.23	61,61,61,61	0
57	MG	1A	4184	1/1	0.96	0.15	21,21,21,21	0
57	MG	1A	3194	1/1	0.96	0.15	41,41,41,41	0
57	MG	2A	3579	1/1	0.96	0.10	28,28,28,28	0
57	MG	2a	3080	1/1	0.96	0.13	33,33,33,33	0
57	MG	1A	3639	1/1	0.96	0.19	31,31,31,31	0
57	MG	2A	3052	1/1	0.96	0.14	33,33,33,33	0
57	MG	1A	3342	1/1	0.96	0.17	41,41,41,41	0
57	MG	1A	3472	1/1	0.96	0.12	51,51,51,51	0
57	MG	1A	3146	1/1	0.96	0.17	29,29,29,29	0
57	MG	2A	3029	1/1	0.96	0.33	42,42,42,42	0
57	MG	2A	3705	1/1	0.96	0.13	29,29,29,29	0
57	MG	2A	3883	1/1	0.96	0.12	39,39,39,39	0
57	MG	2A	3160	1/1	0.96	0.17	44,44,44,44	0
57	MG	2A	3297	1/1	0.96	0.11	51,51,51,51	0
57	MG	2A	3911	1/1	0.96	0.11	61,61,61,61	0
57	MG	1A	3614	1/1	0.96	0.17	43,43,43,43	0
57	MG	1A	3067	1/1	0.96	0.22	31,31,31,31	0
57	MG	2A	3821	1/1	0.96	0.11	45,45,45,45	0
57	MG	1a	3139	1/1	0.96	0.32	35,35,35,35	0
57	MG	1A	3070	1/1	0.96	0.18	26,26,26,26	0
57	MG	1a	3112	1/1	0.96	0.12	46,46,46,46	0
57	MG	2A	3596	1/1	0.96	0.12	40,40,40,40	0
57	MG	2A	3598	1/1	0.96	0.39	53,53,53,53	0
57	MG	1A	4290	1/1	0.96	0.15	59,59,59,59	0
57	MG	1A	3833	1/1	0.96	0.19	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3532	1/1	0.96	0.17	35,35,35,35	0
57	MG	1A	4188	1/1	0.96	0.16	35,35,35,35	0
57	MG	2a	3251	1/1	0.96	0.16	51,51,51,51	0
57	MG	2A	3031	1/1	0.96	0.17	32,32,32,32	0
57	MG	1A	4243	1/1	0.96	0.15	17,17,17,17	0
57	MG	1a	3080	1/1	0.96	0.08	42,42,42,42	0
57	MG	2A	3332	1/1	0.96	0.25	60,60,60,60	0
57	MG	1A	3716	1/1	0.96	0.13	21,21,21,21	0
57	MG	1A	3013	1/1	0.96	0.21	21,21,21,21	0
57	MG	1A	3131	1/1	0.96	0.14	29,29,29,29	0
57	MG	2A	3535	1/1	0.96	0.15	49,49,49,49	0
57	MG	1A	3839	1/1	0.96	0.12	37,37,37,37	0
57	MG	1A	4130	1/1	0.96	0.21	21,21,21,21	0
57	MG	2A	3895	1/1	0.96	0.22	36,36,36,36	0
57	MG	2A	3944	1/1	0.96	0.19	41,41,41,41	0
57	MG	1A	3133	1/1	0.96	0.38	38,38,38,38	0
57	MG	1a	3149	1/1	0.96	0.31	46,46,46,46	0
57	MG	2a	3073	1/1	0.96	0.11	47,47,47,47	0
57	MG	1A	4240	1/1	0.96	0.12	39,39,39,39	0
57	MG	1A	4179	1/1	0.96	0.12	38,38,38,38	0
57	MG	2A	3024	1/1	0.96	0.17	29,29,29,29	0
57	MG	2a	3008	1/1	0.96	0.15	58,58,58,58	0
57	MG	1A	3367	1/1	0.96	0.39	33,33,33,33	0
57	MG	2A	3808	1/1	0.96	0.09	49,49,49,49	0
57	MG	1A	3892	1/1	0.96	0.22	37,37,37,37	0
57	MG	2A	3066	1/1	0.96	0.29	55,55,55,55	0
57	MG	1a	3021	1/1	0.96	0.11	40,40,40,40	0
57	MG	1A	4042	1/1	0.96	0.12	23,23,23,23	0
57	MG	1A	3046	1/1	0.96	0.14	29,29,29,29	0
57	MG	2A	3073	1/1	0.96	0.24	45,45,45,45	0
57	MG	2A	3105	1/1	0.96	0.16	47,47,47,47	0
57	MG	1A	3596	1/1	0.96	0.38	33,33,33,33	0
57	MG	2A	3878	1/1	0.96	0.06	56,56,56,56	0
57	MG	1A	3497	1/1	0.96	0.19	29,29,29,29	0
57	MG	2A	3306	1/1	0.96	0.09	51,51,51,51	0
57	MG	1A	3891	1/1	0.96	0.14	34,34,34,34	0
57	MG	2A	3659	1/1	0.96	0.13	48,48,48,48	0
57	MG	1A	4172	1/1	0.96	0.14	52,52,52,52	0
57	MG	1a	3081	1/1	0.96	0.09	48,48,48,48	0
57	MG	2A	3265	1/1	0.96	0.12	39,39,39,39	0
57	MG	1A	3255	1/1	0.96	0.15	27,27,27,27	0
57	MG	1A	3775	1/1	0.96	0.14	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3498	1/1	0.96	0.13	36,36,36,36	0
57	MG	1A	3751	1/1	0.96	0.16	39,39,39,39	0
57	MG	1A	3651	1/1	0.96	0.17	41,41,41,41	0
57	MG	2A	3200	1/1	0.96	0.18	47,47,47,47	0
57	MG	1A	4018	1/1	0.96	0.19	34,34,34,34	0
57	MG	2A	3239	1/1	0.96	0.20	36,36,36,36	0
57	MG	2A	3752	1/1	0.96	0.12	44,44,44,44	0
57	MG	1a	3194	1/1	0.96	0.09	43,43,43,43	0
57	MG	2A	3955	1/1	0.96	0.36	61,61,61,61	0
57	MG	2A	3182	1/1	0.96	0.19	28,28,28,28	0
57	MG	2A	3884	1/1	0.96	0.10	45,45,45,45	0
57	MG	2A	3935	1/1	0.96	0.17	50,50,50,50	0
57	MG	2A	3642	1/1	0.96	0.11	68,68,68,68	0
57	MG	1A	3091	1/1	0.96	0.23	34,34,34,34	0
57	MG	1A	3715	1/1	0.96	0.13	42,42,42,42	0
57	MG	2A	3824	1/1	0.96	0.16	47,47,47,47	0
57	MG	1A	3140	1/1	0.96	0.15	21,21,21,21	0
57	MG	1A	3192	1/1	0.96	0.11	27,27,27,27	0
57	MG	1A	3635	1/1	0.96	0.23	26,26,26,26	0
57	MG	2A	3751	1/1	0.96	0.13	29,29,29,29	0
57	MG	1A	3071	1/1	0.96	0.09	36,36,36,36	0
57	MG	2A	3166	1/1	0.96	0.12	28,28,28,28	0
57	MG	1A	4222	1/1	0.96	0.19	51,51,51,51	0
57	MG	2a	3077	1/1	0.96	0.17	43,43,43,43	0
58	K	2A	3484	1/1	0.96	0.13	40,40,40,40	0
57	MG	1A	3763	1/1	0.96	0.13	32,32,32,32	0
57	MG	1A	3034	1/1	0.96	0.18	22,22,22,22	0
57	MG	1A	3810	1/1	0.96	0.07	37,37,37,37	0
57	MG	1A	3206	1/1	0.96	0.24	28,28,28,28	0
57	MG	1A	3318	1/1	0.96	0.31	52,52,52,52	0
57	MG	2a	3270	1/1	0.96	0.15	61,61,61,61	0
57	MG	1A	3935	1/1	0.96	0.18	10,10,10,10	0
57	MG	1A	3328	1/1	0.96	0.27	40,40,40,40	0
57	MG	2a	3243	1/1	0.96	0.17	46,46,46,46	0
57	MG	2A	3453	1/1	0.96	0.31	50,50,50,50	0
57	MG	1A	4152	1/1	0.96	0.13	17,17,17,17	0
57	MG	1a	3135	1/1	0.96	0.17	72,72,72,72	0
57	MG	1A	3204	1/1	0.96	0.32	31,31,31,31	0
57	MG	2a	3075	1/1	0.96	0.11	53,53,53,53	0
57	MG	1A	3112	1/1	0.96	0.20	21,21,21,21	0
57	MG	2A	3757	1/1	0.96	0.16	42,42,42,42	0
57	MG	1A	3807	1/1	0.96	0.16	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	4258	1/1	0.96	0.16	42,42,42,42	0
57	MG	2A	3803	1/1	0.96	0.19	43,43,43,43	0
57	MG	1A	3951	1/1	0.96	0.14	29,29,29,29	0
57	MG	2a	3255	1/1	0.96	0.16	45,45,45,45	0
57	MG	1A	3804	1/1	0.96	0.14	31,31,31,31	0
57	MG	2A	3696	1/1	0.96	0.20	51,51,51,51	0
57	MG	2a	3239	1/1	0.96	0.27	53,53,53,53	0
57	MG	1A	3954	1/1	0.96	0.12	46,46,46,46	0
57	MG	1A	3414	1/1	0.96	0.20	35,35,35,35	0
57	MG	1A	3170	1/1	0.96	0.34	33,33,33,33	0
57	MG	2a	3130	1/1	0.96	0.26	47,47,47,47	0
57	MG	1A	4011	1/1	0.96	0.20	31,31,31,31	0
57	MG	1A	3173	1/1	0.96	0.20	26,26,26,26	0
57	MG	2A	3960	1/1	0.96	0.22	37,37,37,37	0
57	MG	2a	3115	1/1	0.96	0.15	61,61,61,61	0
57	MG	1A	4110	1/1	0.96	0.20	38,38,38,38	0
57	MG	2A	3563	1/1	0.96	0.15	53,53,53,53	0
57	MG	1A	3015	1/1	0.96	0.10	21,21,21,21	0
57	MG	1A	3682	1/1	0.96	0.09	29,29,29,29	0
57	MG	2A	3225	1/1	0.96	0.17	43,43,43,43	0
57	MG	1A	3921	1/1	0.96	0.15	40,40,40,40	0
57	MG	1A	3164	1/1	0.96	0.22	26,26,26,26	0
57	MG	1A	4133	1/1	0.96	0.16	15,15,15,15	0
57	MG	2A	3633	1/1	0.96	0.10	57,57,57,57	0
59	ZN	2n	501	1/1	0.96	0.11	79,79,79,79	0
57	MG	1A	3254	1/1	0.96	0.24	36,36,36,36	0
57	MG	1A	4043	1/1	0.96	0.12	47,47,47,47	0
57	MG	1A	3229	1/1	0.96	0.28	36,36,36,36	0
57	MG	2A	3508	1/1	0.96	0.14	41,41,41,41	0
57	MG	1A	3707	1/1	0.96	0.18	31,31,31,31	0
57	MG	1A	3669	1/1	0.96	0.19	36,36,36,36	0
57	MG	1A	3456	1/1	0.96	0.20	41,41,41,41	0
57	MG	1a	3130	1/1	0.96	0.18	33,33,33,33	0
57	MG	1A	3773	1/1	0.96	0.15	27,27,27,27	0
57	MG	2A	3601	1/1	0.96	0.27	46,46,46,46	0
57	MG	1A	3542	1/1	0.96	0.16	22,22,22,22	0
57	MG	2A	3513	1/1	0.96	0.19	38,38,38,38	0
57	MG	1a	3089	1/1	0.96	0.10	57,57,57,57	0
57	MG	1A	3919	1/1	0.96	0.17	14,14,14,14	0
57	MG	1A	3813	1/1	0.96	0.14	10,10,10,10	0
57	MG	2A	3529	1/1	0.96	0.27	45,45,45,45	0
57	MG	1A	3877	1/1	0.96	0.11	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	3134	1/1	0.96	0.24	34,34,34,34	0
57	MG	1A	3628	1/1	0.96	0.24	16,16,16,16	0
57	MG	1a	3212	1/1	0.96	0.13	45,45,45,45	0
57	MG	2A	3619	1/1	0.96	0.15	39,39,39,39	0
57	MG	2A	3251	1/1	0.96	0.10	35,35,35,35	0
57	MG	1A	3960	1/1	0.96	0.13	31,31,31,31	0
57	MG	2A	3140	1/1	0.96	0.17	52,52,52,52	0
57	MG	1A	4146	1/1	0.96	0.16	16,16,16,16	0
57	MG	1A	3072	1/1	0.96	0.22	19,19,19,19	0
57	MG	2A	3958	1/1	0.96	0.14	46,46,46,46	0
58	K	1A	3602	1/1	0.96	0.16	24,24,24,24	0
57	MG	1A	3065	1/1	0.96	0.20	34,34,34,34	0
57	MG	1A	3517	1/1	0.96	0.18	42,42,42,42	0
57	MG	1a	3008	1/1	0.96	0.16	45,45,45,45	0
57	MG	1A	3990	1/1	0.96	0.22	45,45,45,45	0
57	MG	1A	3037	1/1	0.96	0.08	28,28,28,28	0
57	MG	2A	3926	1/1	0.96	0.24	64,64,64,64	0
57	MG	1A	3825	1/1	0.96	0.15	48,48,48,48	0
57	MG	1A	3403	1/1	0.96	0.21	27,27,27,27	0
57	MG	1A	3782	1/1	0.96	0.11	62,62,62,62	0
57	MG	1A	3007	1/1	0.96	0.12	29,29,29,29	0
57	MG	2A	3333	1/1	0.96	0.15	55,55,55,55	0
57	MG	1A	3089	1/1	0.96	0.75	26,26,26,26	0
57	MG	2a	3033	1/1	0.96	0.19	50,50,50,50	0
57	MG	1A	4153	1/1	0.97	0.19	23,23,23,23	0
57	MG	1A	3868	1/1	0.97	0.21	36,36,36,36	0
57	MG	2A	3197	1/1	0.97	0.10	52,52,52,52	0
57	MG	2A	3106	1/1	0.97	0.09	30,30,30,30	0
57	MG	1A	3295	1/1	0.97	0.23	39,39,39,39	0
57	MG	1A	3769	1/1	0.97	0.09	13,13,13,13	0
57	MG	1A	3373	1/1	0.97	0.10	22,22,22,22	0
57	MG	1A	3636	1/1	0.97	0.20	29,29,29,29	0
57	MG	1A	4198	1/1	0.97	0.15	9,9,9,9	0
57	MG	1a	3010	1/1	0.97	0.14	57,57,57,57	0
57	MG	1A	3259	1/1	0.97	0.56	35,35,35,35	0
57	MG	1A	3144	1/1	0.97	0.14	18,18,18,18	0
57	MG	1A	3010	1/1	0.97	0.20	29,29,29,29	0
57	MG	1a	3179	1/1	0.97	0.15	42,42,42,42	0
57	MG	1A	3372	1/1	0.97	0.13	29,29,29,29	0
57	MG	1A	3453	1/1	0.97	0.18	38,38,38,38	0
57	MG	1A	3421	1/1	0.97	0.22	30,30,30,30	0
57	MG	1A	3301	1/1	0.97	0.16	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3469	1/1	0.97	0.28	40,40,40,40	0
57	MG	2A	3428	1/1	0.97	0.26	34,34,34,34	0
57	MG	2a	3113	1/1	0.97	0.16	50,50,50,50	0
57	MG	1A	3004	1/1	0.97	0.13	18,18,18,18	0
57	MG	1A	3128	1/1	0.97	0.16	19,19,19,19	0
57	MG	2A	3389	1/1	0.97	0.14	50,50,50,50	0
57	MG	1A	4010	1/1	0.97	0.12	43,43,43,43	0
57	MG	1A	3629	1/1	0.97	0.16	24,24,24,24	0
57	MG	2a	3167	1/1	0.97	0.18	55,55,55,55	0
57	MG	2A	3722	1/1	0.97	0.10	54,54,54,54	0
57	MG	2A	3448	1/1	0.97	0.34	43,43,43,43	0
57	MG	1A	3457	1/1	0.97	0.19	43,43,43,43	0
57	MG	2A	3362	1/1	0.97	0.10	47,47,47,47	0
57	MG	2A	3522	1/1	0.97	0.14	41,41,41,41	0
57	MG	1A	3632	1/1	0.97	0.13	31,31,31,31	0
57	MG	1A	3374	1/1	0.97	0.12	20,20,20,20	0
57	MG	1a	3086	1/1	0.97	0.20	55,55,55,55	0
57	MG	2A	3823	1/1	0.97	0.10	48,48,48,48	0
57	MG	1A	3157	1/1	0.97	0.29	31,31,31,31	0
57	MG	1A	3169	1/1	0.97	0.23	21,21,21,21	0
57	MG	1A	4080	1/1	0.97	0.17	31,31,31,31	0
57	MG	1A	3347	1/1	0.97	0.28	26,26,26,26	0
57	MG	1A	3729	1/1	0.97	0.22	22,22,22,22	0
57	MG	1A	4027	1/1	0.97	0.20	19,19,19,19	0
57	MG	2A	3663	1/1	0.97	0.13	26,26,26,26	0
57	MG	2A	3499	1/1	0.97	0.17	20,20,20,20	0
57	MG	1A	3168	1/1	0.97	0.16	17,17,17,17	0
57	MG	1A	3396	1/1	0.97	0.26	34,34,34,34	0
57	MG	1A	3231	1/1	0.97	0.21	31,31,31,31	0
57	MG	2A	3689	1/1	0.97	0.16	48,48,48,48	0
57	MG	1A	3617	1/1	0.97	0.14	13,13,13,13	0
57	MG	2A	3637	1/1	0.97	0.14	35,35,35,35	0
57	MG	2A	3716	1/1	0.97	0.15	37,37,37,37	0
57	MG	1A	4001	1/1	0.97	0.17	23,23,23,23	0
57	MG	2A	3947	1/1	0.97	0.14	45,45,45,45	0
57	MG	1a	3102	1/1	0.97	0.16	54,54,54,54	0
57	MG	2a	3152	1/1	0.97	0.10	55,55,55,55	0
57	MG	1A	3220	1/1	0.97	0.18	24,24,24,24	0
57	MG	2A	3834	1/1	0.97	0.11	51,51,51,51	0
57	MG	1A	3208	1/1	0.97	0.20	33,33,33,33	0
57	MG	2A	3622	1/1	0.97	0.25	44,44,44,44	0
57	MG	2a	3208	1/1	0.97	0.07	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3905	1/1	0.97	0.17	21,21,21,21	0
57	MG	1A	3417	1/1	0.97	0.17	25,25,25,25	0
57	MG	2A	3520	1/1	0.97	0.16	52,52,52,52	0
57	MG	1A	3740	1/1	0.97	0.20	38,38,38,38	0
57	MG	1A	3541	1/1	0.97	0.14	39,39,39,39	0
57	MG	2A	3591	1/1	0.97	0.08	33,33,33,33	0
57	MG	2A	3344	1/1	0.97	0.17	34,34,34,34	0
57	MG	1a	3038	1/1	0.97	0.28	38,38,38,38	0
57	MG	2A	3592	1/1	0.97	0.12	43,43,43,43	0
57	MG	1a	3051	1/1	0.97	0.15	36,36,36,36	0
57	MG	1A	3404	1/1	0.97	0.17	30,30,30,30	0
57	MG	1A	3965	1/1	0.97	0.17	31,31,31,31	0
57	MG	2A	3661	1/1	0.97	0.23	41,41,41,41	0
57	MG	1A	4028	1/1	0.97	0.19	24,24,24,24	0
57	MG	2A	3124	1/1	0.97	0.23	36,36,36,36	0
57	MG	2A	3398	1/1	0.97	0.23	54,54,54,54	0
57	MG	1A	3005	1/1	0.97	0.17	32,32,32,32	0
57	MG	1A	4273	1/1	0.97	0.18	30,30,30,30	0
57	MG	2A	3409	1/1	0.97	0.14	50,50,50,50	0
57	MG	1A	3871	1/1	0.97	0.18	15,15,15,15	0
57	MG	2a	3136	1/1	0.97	0.12	62,62,62,62	0
57	MG	1A	3911	1/1	0.97	0.18	26,26,26,26	0
57	MG	1A	3929	1/1	0.97	0.12	30,30,30,30	0
57	MG	1A	3371	1/1	0.97	0.27	20,20,20,20	0
57	MG	1A	3778	1/1	0.97	0.17	49,49,49,49	0
57	MG	1A	3553	1/1	0.97	0.25	31,31,31,31	0
57	MG	2A	3576	1/1	0.97	0.17	32,32,32,32	0
57	MG	2A	3820	1/1	0.97	0.24	59,59,59,59	0
57	MG	1A	3978	1/1	0.97	0.12	53,53,53,53	0
57	MG	1A	3950	1/1	0.97	0.18	46,46,46,46	0
57	MG	1a	3087	1/1	0.97	0.10	57,57,57,57	0
57	MG	2A	3115	1/1	0.97	0.13	43,43,43,43	0
57	MG	2A	3853	1/1	0.97	0.05	37,37,37,37	0
57	MG	2A	3795	1/1	0.97	0.14	24,24,24,24	0
57	MG	1A	3125	1/1	0.97	0.23	33,33,33,33	0
57	MG	1A	3897	1/1	0.97	0.20	41,41,41,41	0
57	MG	2A	3829	1/1	0.97	0.11	39,39,39,39	0
57	MG	2a	3103	1/1	0.97	0.14	39,39,39,39	0
57	MG	2a	3084	1/1	0.97	0.18	53,53,53,53	0
57	MG	1a	3096	1/1	0.97	0.23	40,40,40,40	0
57	MG	2A	3802	1/1	0.97	0.17	53,53,53,53	0
57	MG	1A	3627	1/1	0.97	0.17	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	4049	1/1	0.97	0.15	45,45,45,45	0
57	MG	1A	3054	1/1	0.97	0.21	36,36,36,36	0
57	MG	1A	3854	1/1	0.97	0.15	10,10,10,10	0
57	MG	1A	3972	1/1	0.97	0.18	48,48,48,48	0
57	MG	1A	3623	1/1	0.97	0.25	23,23,23,23	0
57	MG	1A	3937	1/1	0.97	0.17	22,22,22,22	0
57	MG	2A	3942	1/1	0.97	0.07	43,43,43,43	0
57	MG	2A	3503	1/1	0.97	0.27	35,35,35,35	0
57	MG	1A	4285	1/1	0.97	0.20	51,51,51,51	0
57	MG	2A	3949	1/1	0.97	0.08	49,49,49,49	0
57	MG	2A	3131	1/1	0.97	0.21	30,30,30,30	0
57	MG	2A	3666	1/1	0.97	0.11	38,38,38,38	0
57	MG	1A	3961	1/1	0.97	0.10	21,21,21,21	0
57	MG	1a	3065	1/1	0.97	0.21	41,41,41,41	0
57	MG	1A	3785	1/1	0.97	0.21	20,20,20,20	0
57	MG	2A	3534	1/1	0.97	0.22	43,43,43,43	0
57	MG	1A	3504	1/1	0.97	0.25	40,40,40,40	0
57	MG	2a	3045	1/1	0.97	0.21	55,55,55,55	0
57	MG	2a	3221	1/1	0.97	0.20	53,53,53,53	0
57	MG	2A	3760	1/1	0.97	0.15	44,44,44,44	0
57	MG	1A	3336	1/1	0.97	0.23	38,38,38,38	0
57	MG	1a	3206	1/1	0.97	0.15	50,50,50,50	0
57	MG	2A	3909	1/1	0.97	0.17	31,31,31,31	0
57	MG	2A	3691	1/1	0.97	0.11	36,36,36,36	0
57	MG	1a	3068	1/1	0.97	0.13	60,60,60,60	0
57	MG	1A	3766	1/1	0.97	0.12	43,43,43,43	0
57	MG	1A	3227	1/1	0.97	0.15	23,23,23,23	0
57	MG	2a	3227	1/1	0.97	0.20	61,61,61,61	0
57	MG	1A	3841	1/1	0.97	0.15	23,23,23,23	0
57	MG	1A	4270	1/1	0.97	0.06	24,24,24,24	0
57	MG	1A	4246	1/1	0.97	0.09	56,56,56,56	0
57	MG	1A	3966	1/1	0.97	0.16	30,30,30,30	0
57	MG	2A	3919	1/1	0.97	0.14	35,35,35,35	0
57	MG	2a	3280	1/1	0.97	0.15	60,60,60,60	0
57	MG	1A	3637	1/1	0.97	0.16	43,43,43,43	0
57	MG	1A	3009	1/1	0.97	0.14	17,17,17,17	0
57	MG	2a	3108	1/1	0.97	0.22	52,52,52,52	0
57	MG	1A	4008	1/1	0.97	0.19	16,16,16,16	0
57	MG	1A	3236	1/1	0.97	0.16	34,34,34,34	0
57	MG	2A	3694	1/1	0.97	0.18	49,49,49,49	0
57	MG	2a	3143	1/1	0.97	0.14	50,50,50,50	0
57	MG	2A	3956	1/1	0.97	0.20	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	3017	1/1	0.97	0.13	39,39,39,39	0
57	MG	1A	3665	1/1	0.97	0.19	33,33,33,33	0
57	MG	2A	3837	1/1	0.97	0.15	49,49,49,49	0
57	MG	1A	3812	1/1	0.97	0.23	19,19,19,19	0
57	MG	2A	3142	1/1	0.97	0.39	37,37,37,37	0
57	MG	1A	3145	1/1	0.97	0.15	28,28,28,28	0
57	MG	2A	3800	1/1	0.97	0.17	50,50,50,50	0
57	MG	2A	3525	1/1	0.97	0.34	43,43,43,43	0
57	MG	1a	3210	1/1	0.97	0.10	52,52,52,52	0
57	MG	2a	3188	1/1	0.97	0.16	48,48,48,48	0
57	MG	1a	3167	1/1	0.97	0.19	35,35,35,35	0
57	MG	1A	4157	1/1	0.97	0.13	31,31,31,31	0
57	MG	2A	3755	1/1	0.97	0.17	47,47,47,47	0
57	MG	1A	4216	1/1	0.97	0.09	37,37,37,37	0
57	MG	2A	3133	1/1	0.97	0.13	41,41,41,41	0
57	MG	1A	3033	1/1	0.97	0.17	21,21,21,21	0
57	MG	1A	3205	1/1	0.97	0.11	39,39,39,39	0
57	MG	2A	3086	1/1	0.97	0.18	35,35,35,35	0
57	MG	2A	3851	1/1	0.97	0.11	44,44,44,44	0
57	MG	1A	3997	1/1	0.97	0.20	24,24,24,24	0
57	MG	1A	3732	1/1	0.97	0.30	64,64,64,64	0
57	MG	2A	3609	1/1	0.97	0.14	44,44,44,44	0
57	MG	1A	3241	1/1	0.97	0.25	38,38,38,38	0
57	MG	2A	3938	1/1	0.97	0.19	44,44,44,44	0
57	MG	1A	3272	1/1	0.97	0.12	24,24,24,24	0
57	MG	1A	4225	1/1	0.97	0.17	33,33,33,33	0
57	MG	2A	3732	1/1	0.97	0.21	49,49,49,49	0
57	MG	1A	3959	1/1	0.97	0.11	33,33,33,33	0
57	MG	1A	4059	1/1	0.97	0.16	29,29,29,29	0
57	MG	2A	3788	1/1	0.97	0.12	45,45,45,45	0
57	MG	2A	3816	1/1	0.97	0.27	36,36,36,36	0
57	MG	1A	4111	1/1	0.97	0.13	31,31,31,31	0
57	MG	2A	3405	1/1	0.97	0.17	42,42,42,42	0
57	MG	2A	3524	1/1	0.97	0.26	34,34,34,34	0
57	MG	1A	3615	1/1	0.97	0.23	37,37,37,37	0
57	MG	1A	3076	1/1	0.97	0.16	9,9,9,9	0
57	MG	2A	3433	1/1	0.97	0.38	39,39,39,39	0
57	MG	2A	3468	1/1	0.97	0.28	41,41,41,41	0
57	MG	1A	4247	1/1	0.97	0.11	45,45,45,45	0
57	MG	1A	3678	1/1	0.97	0.20	19,19,19,19	0
57	MG	1A	3819	1/1	0.97	0.10	51,51,51,51	0
57	MG	1a	3127	1/1	0.97	0.21	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	3530	1/1	0.97	0.15	27,27,27,27	0
57	MG	1A	3148	1/1	0.97	0.18	25,25,25,25	0
57	MG	2a	3237	1/1	0.97	0.12	57,57,57,57	0
57	MG	1A	3592	1/1	0.97	0.24	27,27,27,27	0
57	MG	1a	3016	1/1	0.97	0.19	44,44,44,44	0
57	MG	2a	3017	1/1	0.97	0.15	43,43,43,43	0
57	MG	2A	3152	1/1	0.97	0.23	36,36,36,36	0
57	MG	1A	3866	1/1	0.97	0.16	55,55,55,55	0
57	MG	1A	3509	1/1	0.97	0.14	41,41,41,41	0
57	MG	2A	3473	1/1	0.97	0.30	46,46,46,46	0
57	MG	1A	3364	1/1	0.97	0.10	42,42,42,42	0
57	MG	1A	3811	1/1	0.97	0.20	11,11,11,11	0
57	MG	1A	3836	1/1	0.97	0.21	25,25,25,25	0
57	MG	1A	3591	1/1	0.97	0.15	17,17,17,17	0
57	MG	1A	3944	1/1	0.97	0.09	24,24,24,24	0
57	MG	2A	3246	1/1	0.97	0.14	34,34,34,34	0
57	MG	2A	3822	1/1	0.97	0.10	45,45,45,45	0
57	MG	1A	3703	1/1	0.97	0.23	34,34,34,34	0
57	MG	1A	3519	1/1	0.97	0.08	32,32,32,32	0
57	MG	1A	4058	1/1	0.97	0.17	21,21,21,21	0
57	MG	1A	3110	1/1	0.97	0.15	31,31,31,31	0
57	MG	1A	3191	1/1	0.97	0.21	14,14,14,14	0
57	MG	2A	3442	1/1	0.97	0.15	45,45,45,45	0
57	MG	1A	3712	1/1	0.97	0.15	24,24,24,24	0
57	MG	1a	3119	1/1	0.97	0.20	48,48,48,48	0
57	MG	2A	3470	1/1	0.97	0.18	46,46,46,46	0
57	MG	2A	3179	1/1	0.97	0.16	40,40,40,40	0
57	MG	1A	4064	1/1	0.97	0.12	26,26,26,26	0
57	MG	1A	3012	1/1	0.97	0.15	22,22,22,22	0
57	MG	1A	3900	1/1	0.97	0.18	27,27,27,27	0
57	MG	2A	3887	1/1	0.97	0.16	38,38,38,38	0
57	MG	1A	3298	1/1	0.97	0.21	26,26,26,26	0
57	MG	1A	3368	1/1	0.97	0.11	31,31,31,31	0
57	MG	2A	3873	1/1	0.97	0.16	53,53,53,53	0
57	MG	2A	3838	1/1	0.97	0.11	37,37,37,37	0
57	MG	1A	3028	1/1	0.97	0.07	39,39,39,39	0
57	MG	2a	3145	1/1	0.97	0.15	58,58,58,58	0
57	MG	1A	3969	1/1	0.97	0.12	39,39,39,39	0
57	MG	2A	3172	1/1	0.97	0.19	33,33,33,33	0
57	MG	1A	3571	1/1	0.97	0.27	28,28,28,28	0
57	MG	1A	4084	1/1	0.97	0.13	19,19,19,19	0
57	MG	2a	3139	1/1	0.97	0.17	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	3024	1/1	0.97	0.07	64,64,64,64	0
57	MG	1A	3908	1/1	0.98	0.24	19,19,19,19	0
57	MG	1A	4248	1/1	0.98	0.16	41,41,41,41	0
57	MG	1A	4229	1/1	0.98	0.12	58,58,58,58	0
57	MG	2A	3021	1/1	0.98	0.12	26,26,26,26	0
57	MG	2A	3718	1/1	0.98	0.23	40,40,40,40	0
57	MG	1A	3721	1/1	0.98	0.11	39,39,39,39	0
57	MG	2a	3275	1/1	0.98	0.10	54,54,54,54	0
57	MG	2A	3831	1/1	0.98	0.14	50,50,50,50	0
57	MG	1A	3293	1/1	0.98	0.09	41,41,41,41	0
59	ZN	29	501	1/1	0.98	0.11	59,59,59,59	0
57	MG	1A	3036	1/1	0.98	0.18	20,20,20,20	0
57	MG	2A	3639	1/1	0.98	0.23	33,33,33,33	0
57	MG	1A	3075	1/1	0.98	0.25	25,25,25,25	0
57	MG	1A	4032	1/1	0.98	0.12	29,29,29,29	0
57	MG	1A	3625	1/1	0.98	0.24	22,22,22,22	0
57	MG	1A	3673	1/1	0.98	0.18	22,22,22,22	0
57	MG	1A	3907	1/1	0.98	0.18	20,20,20,20	0
57	MG	1a	3045	1/1	0.98	0.15	38,38,38,38	0
57	MG	1A	3688	1/1	0.98	0.23	33,33,33,33	0
57	MG	1A	3958	1/1	0.98	0.21	26,26,26,26	0
57	MG	1A	3407	1/1	0.98	0.18	43,43,43,43	0
57	MG	2A	3583	1/1	0.98	0.21	36,36,36,36	0
57	MG	1A	3177	1/1	0.98	0.10	23,23,23,23	0
57	MG	2A	3604	1/1	0.98	0.21	34,34,34,34	0
57	MG	1A	3898	1/1	0.98	0.13	18,18,18,18	0
57	MG	2A	3672	1/1	0.98	0.16	50,50,50,50	0
57	MG	1A	3670	1/1	0.98	0.16	30,30,30,30	0
57	MG	1A	3039	1/1	0.98	0.20	16,16,16,16	0
57	MG	1A	3102	1/1	0.98	0.19	20,20,20,20	0
57	MG	1A	3633	1/1	0.98	0.13	40,40,40,40	0
57	MG	1A	4155	1/1	0.98	0.23	23,23,23,23	0
57	MG	2A	3936	1/1	0.98	0.19	30,30,30,30	0
57	MG	1A	3025	1/1	0.98	0.28	16,16,16,16	0
57	MG	1A	3331	1/1	0.98	0.23	34,34,34,34	0
57	MG	1A	3207	1/1	0.98	0.19	19,19,19,19	0
57	MG	1A	3038	1/1	0.98	0.15	29,29,29,29	0
57	MG	1A	4165	1/1	0.98	0.10	28,28,28,28	0
57	MG	1A	3181	1/1	0.98	0.15	41,41,41,41	0
57	MG	1A	3011	1/1	0.98	0.17	27,27,27,27	0
57	MG	1A	3622	1/1	0.98	0.18	31,31,31,31	0
57	MG	1a	3126	1/1	0.98	0.20	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	3189	1/1	0.98	0.19	17,17,17,17	0
57	MG	1A	4056	1/1	0.98	0.12	25,25,25,25	0
57	MG	1A	3749	1/1	0.98	0.11	40,40,40,40	0
57	MG	1A	3491	1/1	0.98	0.14	33,33,33,33	0
57	MG	2A	3141	1/1	0.98	0.20	34,34,34,34	0
57	MG	1A	3132	1/1	0.98	0.65	36,36,36,36	0
57	MG	1A	3760	1/1	0.98	0.19	23,23,23,23	0
57	MG	1A	3238	1/1	0.98	0.15	35,35,35,35	0
57	MG	1A	3603	1/1	0.98	0.18	37,37,37,37	0
57	MG	1A	4156	1/1	0.98	0.14	19,19,19,19	0
57	MG	1A	3213	1/1	0.98	0.23	33,33,33,33	0
57	MG	2A	3414	1/1	0.98	0.24	56,56,56,56	0
59	ZN	25	501	1/1	0.98	0.19	52,52,52,52	0
57	MG	1A	4269	1/1	0.98	0.14	38,38,38,38	0
57	MG	1A	3188	1/1	0.98	0.25	27,27,27,27	0
57	MG	2A	3153	1/1	0.98	0.14	30,30,30,30	0
57	MG	1A	3352	1/1	0.98	0.22	35,35,35,35	0
57	MG	1A	3982	1/1	0.98	0.22	50,50,50,50	0
57	MG	1A	3257	1/1	0.98	0.24	20,20,20,20	0
57	MG	1A	3735	1/1	0.98	0.10	48,48,48,48	0
57	MG	2A	3290	1/1	0.98	0.20	40,40,40,40	0
57	MG	1A	3699	1/1	0.98	0.27	35,35,35,35	0
57	MG	1a	3115	1/1	0.98	0.13	55,55,55,55	0
57	MG	1A	3187	1/1	0.98	0.14	18,18,18,18	0
57	MG	1A	4046	1/1	0.98	0.20	35,35,35,35	0
57	MG	2A	3852	1/1	0.98	0.08	44,44,44,44	0
59	ZN	1Y	501	1/1	0.98	0.15	56,56,56,56	0
57	MG	1A	4144	1/1	0.98	0.13	11,11,11,11	0
57	MG	1A	4242	1/1	0.98	0.09	27,27,27,27	0
57	MG	1A	4015	1/1	0.98	0.14	26,26,26,26	0
57	MG	1A	3162	1/1	0.98	0.16	23,23,23,23	0
57	MG	1A	4016	1/1	0.98	0.21	32,32,32,32	0
57	MG	1A	3418	1/1	0.98	0.19	19,19,19,19	0
57	MG	1A	3884	1/1	0.98	0.16	12,12,12,12	0
57	MG	2A	3040	1/1	0.98	0.21	21,21,21,21	0
57	MG	1a	3208	1/1	0.98	0.14	34,34,34,34	0
57	MG	1A	3450	1/1	0.98	0.09	56,56,56,56	0
57	MG	2A	3910	1/1	0.98	0.15	18,18,18,18	0
57	MG	1a	3169	1/1	0.98	0.12	35,35,35,35	0
57	MG	2A	3027	1/1	0.98	0.18	37,37,37,37	0
57	MG	2A	3096	1/1	0.98	0.27	40,40,40,40	0
57	MG	2A	3868	1/1	0.98	0.05	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	3962	1/1	0.98	0.16	18,18,18,18	0
57	MG	1A	3676	1/1	0.98	0.18	18,18,18,18	0
57	MG	2a	3260	1/1	0.98	0.13	62,62,62,62	0
57	MG	1A	3437	1/1	0.98	0.24	36,36,36,36	0
60	SF4	1d	501	8/8	0.98	0.14	47,48,61,68	0
57	MG	1A	3594	1/1	0.98	0.12	21,21,21,21	0
57	MG	1A	3756	1/1	0.98	0.22	30,30,30,30	0
57	MG	2a	3175	1/1	0.98	0.16	50,50,50,50	0
57	MG	1A	3392	1/1	0.98	0.13	35,35,35,35	0
57	MG	1A	3283	1/1	0.98	0.21	31,31,31,31	0
57	MG	2a	3241	1/1	0.98	0.19	50,50,50,50	0
57	MG	2A	3025	1/1	0.98	0.21	45,45,45,45	0
57	MG	1A	3415	1/1	0.98	0.32	31,31,31,31	0
57	MG	2A	3425	1/1	0.98	0.10	47,47,47,47	0
57	MG	1A	3933	1/1	0.98	0.16	49,49,49,49	0
57	MG	2A	3744	1/1	0.98	0.10	37,37,37,37	0
57	MG	1A	3956	1/1	0.98	0.14	22,22,22,22	0
57	MG	1A	3913	1/1	0.98	0.13	15,15,15,15	0
57	MG	1A	3003	1/1	0.98	0.21	11,11,11,11	0
57	MG	2A	3614	1/1	0.98	0.12	31,31,31,31	0
57	MG	1A	3783	1/1	0.98	0.27	29,29,29,29	0
57	MG	2A	3454	1/1	0.98	0.15	54,54,54,54	0
57	MG	1A	3620	1/1	0.98	0.20	28,28,28,28	0
57	MG	1A	3723	1/1	0.98	0.20	32,32,32,32	0
57	MG	1A	3024	1/1	0.98	0.30	26,26,26,26	0
57	MG	2A	3920	1/1	0.98	0.12	53,53,53,53	0
57	MG	1A	3948	1/1	0.98	0.22	13,13,13,13	0
57	MG	2A	3155	1/1	0.98	0.12	33,33,33,33	0
57	MG	1a	3188	1/1	0.98	0.10	52,52,52,52	0
57	MG	1A	3381	1/1	0.98	0.14	29,29,29,29	0
59	ZN	1n	501	1/1	0.98	0.17	47,47,47,47	0
57	MG	1A	3051	1/1	0.98	0.14	15,15,15,15	0
57	MG	2A	3581	1/1	0.98	0.18	17,17,17,17	0
57	MG	2A	3903	1/1	0.98	0.12	51,51,51,51	0
57	MG	1A	3154	1/1	0.98	0.16	20,20,20,20	0
57	MG	2A	3365	1/1	0.98	0.31	42,42,42,42	0
57	MG	1a	3155	1/1	0.98	0.15	45,45,45,45	0
57	MG	1A	3179	1/1	0.98	0.19	9,9,9,9	0
59	ZN	26	501	1/1	0.98	0.18	53,53,53,53	0
60	SF4	2d	501	8/8	0.98	0.10	62,69,73,85	0
57	MG	2a	3047	1/1	0.98	0.16	50,50,50,50	0
57	MG	1A	4073	1/1	0.98	0.17	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	1A	4171	1/1	0.98	0.19	49,49,49,49	0
57	MG	2a	3074	1/1	0.98	0.08	58,58,58,58	0
57	MG	1A	3326	1/1	0.98	0.20	23,23,23,23	0
57	MG	2A	3434	1/1	0.98	0.26	40,40,40,40	0
57	MG	1A	3983	1/1	0.98	0.12	36,36,36,36	0
57	MG	1A	3391	1/1	0.98	0.27	24,24,24,24	0
57	MG	2a	3114	1/1	0.98	0.08	55,55,55,55	0
57	MG	1A	3675	1/1	0.98	0.17	31,31,31,31	0
57	MG	2A	3287	1/1	0.98	0.07	48,48,48,48	0
57	MG	1A	3928	1/1	0.98	0.10	32,32,32,32	0
57	MG	2A	3366	1/1	0.98	0.09	33,33,33,33	0
57	MG	1A	3618	1/1	0.98	0.18	28,28,28,28	0
57	MG	2A	3704	1/1	0.98	0.14	30,30,30,30	0
57	MG	1a	3255	1/1	0.98	0.19	44,44,44,44	0
57	MG	1A	3253	1/1	0.98	0.19	20,20,20,20	0
57	MG	2A	3607	1/1	0.98	0.19	37,37,37,37	0
57	MG	1A	4160	1/1	0.98	0.19	23,23,23,23	0
57	MG	1A	3927	1/1	0.98	0.10	35,35,35,35	0
57	MG	1A	3695	1/1	0.98	0.10	34,34,34,34	0
57	MG	1A	3677	1/1	0.98	0.26	21,21,21,21	0
57	MG	1A	3945	1/1	0.98	0.16	16,16,16,16	0
57	MG	2A	3623	1/1	0.98	0.06	63,63,63,63	0
57	MG	2a	3216	1/1	0.98	0.13	56,56,56,56	0
57	MG	1A	3209	1/1	0.98	0.23	22,22,22,22	0
57	MG	1A	3153	1/1	0.98	0.22	26,26,26,26	0
57	MG	1A	3035	1/1	0.98	0.22	19,19,19,19	0
57	MG	1a	3091	1/1	0.98	0.25	45,45,45,45	0
57	MG	1A	3690	1/1	0.98	0.11	27,27,27,27	0
57	MG	1A	3215	1/1	0.98	0.15	18,18,18,18	0
57	MG	2A	3502	1/1	0.98	0.17	25,25,25,25	0
57	MG	1A	3416	1/1	0.99	0.29	21,21,21,21	0
57	MG	1A	3014	1/1	0.99	0.21	17,17,17,17	0
57	MG	1A	3621	1/1	0.99	0.14	32,32,32,32	0
57	MG	1A	3564	1/1	0.99	0.22	36,36,36,36	0
57	MG	2A	3161	1/1	0.99	0.18	29,29,29,29	0
57	MG	2A	3451	1/1	0.99	0.16	41,41,41,41	0
57	MG	1A	4000	1/1	0.99	0.24	30,30,30,30	0
57	MG	2A	3679	1/1	0.99	0.26	43,43,43,43	0
57	MG	1A	3755	1/1	0.99	0.17	7,7,7,7	0
57	MG	1A	3975	1/1	0.99	0.11	25,25,25,25	0
57	MG	1A	4236	1/1	0.99	0.21	10,10,10,10	0
57	MG	1A	3300	1/1	0.99	0.28	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	1A	3914	1/1	0.99	0.17	23,23,23,23	0
57	MG	2A	3847	1/1	0.99	0.16	29,29,29,29	0
57	MG	1A	3114	1/1	0.99	0.22	25,25,25,25	0
57	MG	1A	3044	1/1	0.99	0.19	21,21,21,21	0
57	MG	1A	4203	1/1	0.99	0.18	16,16,16,16	0
57	MG	1A	3043	1/1	0.99	0.18	22,22,22,22	0
57	MG	1A	3687	1/1	0.99	0.34	24,24,24,24	0
57	MG	1A	4237	1/1	0.99	0.18	30,30,30,30	0
57	MG	1A	3694	1/1	0.99	0.19	32,32,32,32	0
57	MG	2A	3782	1/1	0.99	0.14	23,23,23,23	0
57	MG	1A	3762	1/1	0.99	0.22	27,27,27,27	0
57	MG	2A	3650	1/1	0.99	0.17	24,24,24,24	0
57	MG	2A	3698	1/1	0.99	0.15	44,44,44,44	0
57	MG	1A	4158	1/1	0.99	0.17	23,23,23,23	0
59	ZN	15	501	1/1	0.99	0.20	37,37,37,37	0
57	MG	2A	3582	1/1	0.99	0.29	53,53,53,53	0
57	MG	1A	3685	1/1	0.99	0.22	31,31,31,31	0
57	MG	1A	3030	1/1	0.99	0.27	23,23,23,23	0
57	MG	1A	4252	1/1	0.99	0.19	17,17,17,17	0
57	MG	1A	3656	1/1	0.99	0.25	18,18,18,18	0
57	MG	1A	3780	1/1	0.99	0.20	11,11,11,11	0
57	MG	1A	3547	1/1	0.99	0.17	19,19,19,19	0
57	MG	1a	3011	1/1	0.99	0.20	19,19,19,19	0
57	MG	1A	4135	1/1	0.99	0.15	21,21,21,21	0
57	MG	1A	3662	1/1	0.99	0.16	31,31,31,31	0
57	MG	1A	3156	1/1	0.99	0.31	28,28,28,28	0
57	MG	2A	3476	1/1	0.99	0.21	34,34,34,34	0
57	MG	2A	3739	1/1	0.99	0.13	25,25,25,25	0
57	MG	1A	3824	1/1	0.99	0.18	16,16,16,16	0
57	MG	1A	3243	1/1	0.99	0.16	23,23,23,23	0
59	ZN	19	501	1/1	0.99	0.20	35,35,35,35	0
57	MG	2A	3777	1/1	0.99	0.11	41,41,41,41	0
57	MG	2A	3439	1/1	0.99	0.34	47,47,47,47	0
57	MG	1A	3827	1/1	0.99	0.16	19,19,19,19	0
57	MG	2A	3267	1/1	0.99	0.15	44,44,44,44	0
57	MG	1A	4017	1/1	0.99	0.16	27,27,27,27	0
57	MG	1A	3185	1/1	0.99	0.14	21,21,21,21	0
59	ZN	16	501	1/1	0.99	0.19	36,36,36,36	0
57	MG	2a	3228	1/1	0.99	0.11	45,45,45,45	0
57	MG	1A	3842	1/1	0.99	0.13	7,7,7,7	0
57	MG	1A	3410	1/1	0.99	0.18	29,29,29,29	0
57	MG	1A	3838	1/1	0.99	0.19	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	1a	3219	1/1	0.99	0.11	32,32,32,32	0
57	MG	1A	3040	1/1	0.99	0.12	29,29,29,29	0
57	MG	1A	3671	1/1	1.00	0.21	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.