In [ ]:
```
import sys
!{sys.executable} -m pip install --user scikit-allel
```

In [1]:
```
import numpy as np
import scipy
import pandas
import matplotlib as mpl
import matplotlib.pyplot as plt
%matplotlib inline
import seaborn as sns
sns.set_style('white')
sns.set_style('ticks')
sns.set_context('notebook')
import h5py
import allel; print('scikit-allel', allel.__version__)
```

```
scikit-allel 1.3.8
```

VCF to HDF5

In [2]:
```
allel.vcf_to_hdf5('/users/mcevoysu/scratch/output/Pavium/vcf_filtering/ra
```

Get data

In [3]:
```
callset_var_fn = '/users/mcevoysu/scratch/output/Pavium/scikit-allel/raw_
callset_var = h5py.File(callset_var_fn, mode='r')
```

In [4]:
```
calldata_var = callset_var['calldata']
list(calldata_var)
```

Out[4]:
```
['AD', 'DP', 'GQ', 'GT', 'MIN_DP', 'PGT', 'PID', 'PL', 'PS', 'RGQ', 'S
B']
```

In [5]:
```
list(callset_var['variants'])
```

Out[5]:
```
['AC',
 'AF',
 'ALT',
 'AN',
 'BaseQRankSum',
 'CHROM',
 'DP',
 'END',
 'ExcessHet',
 'FILTER_LowQual',
 'FILTER_PASS',
 'FS',
 'ID',
 'InbreedingCoeff',
 'MLEAC',
 'MLEAF',
 'MQ',
 'MQRankSum',
 'POS',
 'QD',
 'QUAL',
 'RAW_MQandDP',
 'REF',
 'ReadPosRankSum',
 'SOR',
 'altlen',
 'is_snp',
 'numalt']
```

Make datasets

In [6]:
```
variants = allel.VariantChunkedTable(callset_var['variants'])
variants
```

Out[6]: <VariantChunkedTable shape=(262360,) dtype=[('AC', '<i4', (3,)), ('AF', '<f4', (3,)), ('ALT', 'O', (3,)), ('AN', '<i4'), ('BaseQRankSum', '<f4'), ('CHROM', 'O'), ('DP', '<i4'), ('END', '<i4'), ('ExcessHet', '<f4'), ('FILTER_LowQual', '?'), ('FILTER_PASS', '?'), ('FS', '<f4'), ('ID', 'O'), ('InbreedingCoeff', '<f4'), ('MLEAC', '<i4', (3,)), ('MLEAF', '<f4', (3,)), ('MQ', '<f4'), ('MQRankSum', '<f4'), ('POS', '<i4'), ('QD', '<f4'), ('QUAL', '<f4'), ('RAW_MQandDP', '<i4', (2,)), ('REF', 'O'), ('ReadPosRankSum', '<f4'), ('SOR', '<f4'), ('altlen', '<i4', (3,)), ('is_snp', '?'), ('numalt', '<i4')] nbytes=44.8M cbytes=9.3M cratio=4.8 values=h5py._hl.group.Group>

	AC	AF	ALT	AN	BaseQRankSum	CHROM	DP	END	ExcessH
0	[4 -1 -1]	[0.007353 nan nan]	[b'C' b'' b'']	542	1.67	b'chr_1'	8776	-1	0.0484
1	[4 -1 -1]	[0.007353 nan nan]	[b'C' b'' b'']	542	1.67	b'chr_1'	8788	-1	0.0484
2	[1 -1 -1]	[0.001838 nan nan]	[b'T' b'' b'']	542	0.82	b'chr_1'	8962	-1	0.0
...									
262357	[2 -1 -1]	[0.003676 nan nan]	[b'A' b'' b'']	542	nan	b'chr_8'	2351	-1	0.0
262358	[1 -1 -1]	[0.001838 nan nan]	[b'A' b'' b'']	542	0.431	b'chr_8'	792	-1	0.0
262359	[1 -1 -1]	[0.001838 nan nan]	[b'T' b'' b'']	542	0.674	b'chr_8'	606	-1	0.0

In [7]:
```
variants_np = variants[:]
rawsnps = variants_np.query('(is_snp == True)')
rawsnps
```

Out[7]: <VariantTable shape=(158592,) dtype=(numpy.record, [('AC', '<i4', (3,)), ('AF', '<f4', (3,)), ('ALT', 'O', (3,)), ('AN', '<i4'), ('BaseQRankSum', '<f4'), ('CHROM', 'O'), ('DP', '<i4'), ('END', '<i4'), ('ExcessHet', '<f4'), ('FILTER_LowQual', '?'), ('FILTER_PASS', '?'), ('FS', '<f4'), ('ID', 'O'), ('InbreedingCoeff', '<f4'), ('MLEAC', '<i4', (3,)), ('MLEAF', '<f4', (3,)), ('MQ', '<f4'), ('MQRankSum', '<f4'), ('POS', '<i4'), ('QD', '<f4'), ('QUAL', '<f4'), ('RAW_MQandDP', '<i4', (2,)), ('REF', 'O'), ('ReadPosRankSum', '<f4'), ('SOR', '<f4'), ('altlen', '<i4', (3,)), ('is_snp', '?'), ('numalt', '<i4')])>

	AC	AF	ALT	AN	BaseQRankSum	CHROM	DP	END	ExcessH
0	[4 -1 -1]	[0.007353 nan nan]	[b'C' b'' b'']	542	1.67	b'chr_1'	8776	-1	0.0484
1	[4 -1 -1]	[0.007353 nan nan]	[b'C' b'' b'']	542	1.67	b'chr_1'	8788	-1	0.0484
2	[1 -1 -1]	[0.001838 nan nan]	[b'T' b'' b'']	542	0.82	b'chr_1'	8962	-1	0.0
...									
158589	[2 -1 -1]	[0.003676 nan nan]	[b'A' b'' b'']	542	nan	b'chr_8'	2351	-1	0.0
158590	[1 -1 -1]	[0.001838 nan nan]	[b'A' b'' b'']	542	0.431	b'chr_8'	792	-1	0.0
158591	[1 -1 -1]	[0.001838 nan nan]	[b'T' b'' b'']	542	0.674	b'chr_8'	606	-1	0.0

In [8]:
```
notsnp = variants_np.query('(is_snp != True)')
notsnp
```

Out[8]: <VariantTable shape=(103768,) dtype=(numpy.record, [('AC', '<i4', (3,)), ('AF', '<f4', (3,)), ('ALT', 'O', (3,)), ('AN', '<i4'), ('BaseQRankSum', '<f4'), ('CHROM', 'O'), ('DP', '<i4'), ('END', '<i4'), ('ExcessHet', '<f4'), ('FILTER_LowQual', '?'), ('FILTER_PASS', '?'), ('FS', '<f4'), ('ID', 'O'), ('InbreedingCoeff', '<f4'), ('MLEAC', '<i4', (3,)), ('MLEAF', '<f4', (3,)), ('MQ', '<f4'), ('MQRankSum', '<f4'), ('POS', '<i4'), ('QD', '<f4'), ('QUAL', '<f4'), ('RAW_MQandDP', '<i4', (2,)), ('REF', 'O'), ('ReadPosRankSum', '<f4'), ('SOR', '<f4'), ('altlen', '<i4', (3,)), ('is_snp', '?'), ('numalt', '<i4')])>

	AC	AF	ALT	AN	BaseQRankSum	CHROM	DP	END	ExcessHe
0	[1 -1 -1]	[0.001838 nan nan]	[b'*' b'' b'']	542	nan	b'chr_1'	8304	-1	0.0
1	[3 -1 -1]	[0.005515 nan nan]	[b'*' b'' b'']	542	nan	b'chr_1'	6012	-1	0.0242
2	[1 -1 -1]	[0.001838 nan nan]	[b'*' b'' b'']	542	0.79	b'chr_1'	8699	-1	0.0
...									
103765	[6 -1 -1]	[0.011 nan nan]	[b'*' b'' b'']	542	nan	b'chr_8'	365	-1	0.0
103766	[6 24 -1]	[0.011 0.044 nan]	[b'*' b'G' b'']	540	0.0	b'chr_8'	358	-1	0.0
103767	[6 -1 -1]	[0.011 nan nan]	[b'*' b'' b'']	542	nan	b'chr_8'	362	-1	0.0

Plot function

In [9]:
```
def plot_hist(f, dsubset='', bins=30, ):
    if dsubset == 'var':
        x = variants[f][:]
        l = 'Variant'
    elif dsubset == 'snp':
        x = rawsnps[f][:]
        l = 'Raw SNP'
    elif dsubset == 'notsnp':
        x = notsnp[f][:]
        l = 'Raw Not SNP'
    elif dsubset == 'biallelic':
        x = biallelic_np[f][:]
        l = 'Biallelic SNP'
    elif dsubset == 'varsel':
        x = var_selection[f][:]
        l = 'Filtered Variants'
    elif dsubset == 'snpsel':
        x = snp_selection[f][:]
        l = 'Filtered SNP'
    else:
```

```
        x = bi_selection[f][:]
        l = 'Biallelic SNP'
    fig, ax = plt.subplots(figsize=(10, 5))
    sns.despine(ax=ax, offset=10)
    ax.hist(x, bins=bins)
    ax.set_xlabel(f)
    ax.set_ylabel('No. variants')
    ax.set_title('%s %s distribution' % (l, f))
```

Find Biallelic SNPS

In [10]:
```
numalt = rawsnps['numalt']
np.max(numalt)
```

Out[10]:
```
3
```

In [11]:
```
count_numalt = np.bincount(numalt)
count_numalt
```

Out[11]:
```
array([     0, 156606,   1959,     27])
```

In [12]:
```
n_multiallelic = np.sum(count_numalt[2:])
n_multiallelic
```

Out[12]:
```
1986
```

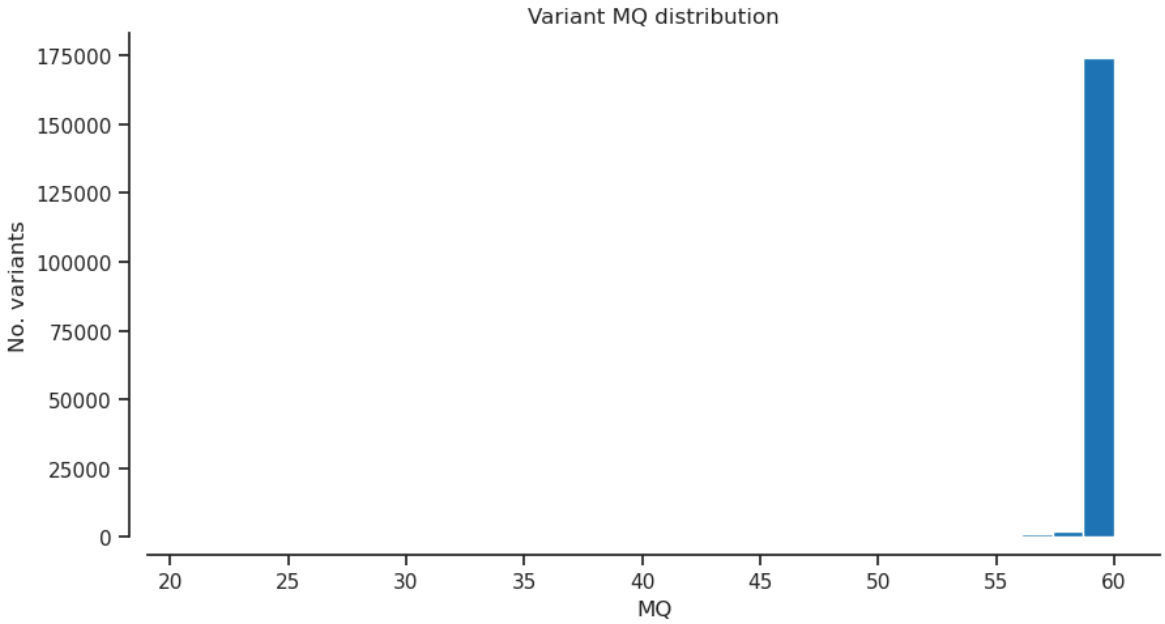
In [13]:
```
filter_expression = '(numalt == 1)'
biallelic_np = rawsnps.query(filter_expression)[:]
biallelic_np
```

Out[13]: <VariantTable shape=(156606,) dtype=(numpy.record, [('AC', '<i4', (3,)), ('AF', '<f4', (3,)), ('ALT', 'O', (3,)), ('AN', '<i4'), ('BaseQRankSum', '<f4'), ('CHROM', 'O'), ('DP', '<i4'), ('END', '<i4'), ('ExcessHet', '<f4'), ('FILTER_LowQual', '?'), ('FILTER_PASS', '?'), ('FS', '<f4'), ('ID', 'O'), ('InbreedingCoeff', '<f4'), ('MLEAC', '<i4', (3,)), ('MLEAF', '<f4', (3,)), ('MQ', '<f4'), ('MQRankSum', '<f4'), ('POS', '<i4'), ('QD', '<f4'), ('QUAL', '<f4'), ('RAW_MQandDP', '<i4', (2,)), ('REF', 'O'), ('ReadPosRankSum', '<f4'), ('SOR', '<f4'), ('altlen', '<i4', (3,)), ('is_snp', '?'), ('numalt', '<i4')])>

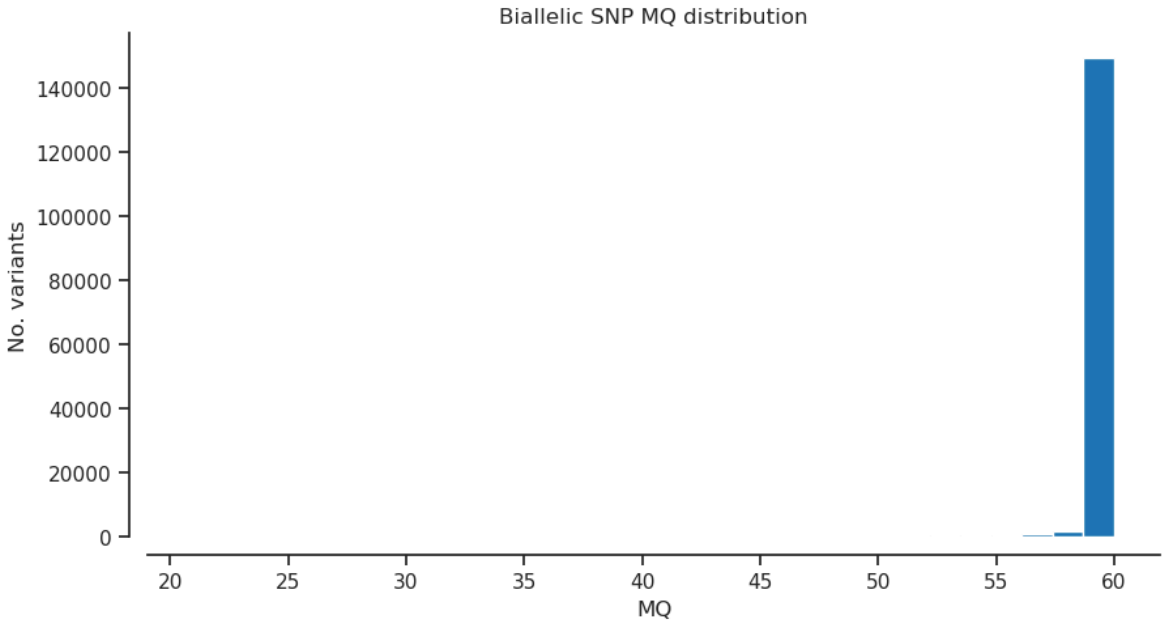
	AC	AF	ALT	AN	BaseQRankSum	CHROM	DP	END	ExcessH
0	[4 -1 -1]	[0.007353 nan nan]	[b'C' b'' b'']	542	1.67	b'chr_1'	8776	-1	0.0484
1	[4 -1 -1]	[0.007353 nan nan]	[b'C' b'' b'']	542	1.67	b'chr_1'	8788	-1	0.0484
2	[1 -1 -1]	[0.001838 nan nan]	[b'T' b'' b'']	542	0.82	b'chr_1'	8962	-1	0.0
...									
156603	[2 -1 -1]	[0.003676 nan nan]	[b'A' b'' b'']	542	nan	b'chr_8'	2351	-1	0.0
156604	[1 -1 -1]	[0.001838 nan nan]	[b'A' b'' b'']	542	0.431	b'chr_8'	792	-1	0.0
156605	[1 -1 -1]	[0.001838 nan nan]	[b'T' b'' b'']	542	0.674	b'chr_8'	606	-1	0.0

MQ - RMS mapping quality

In [14]:
```
plot_hist('MQ','var') # RMS mapping quality
```

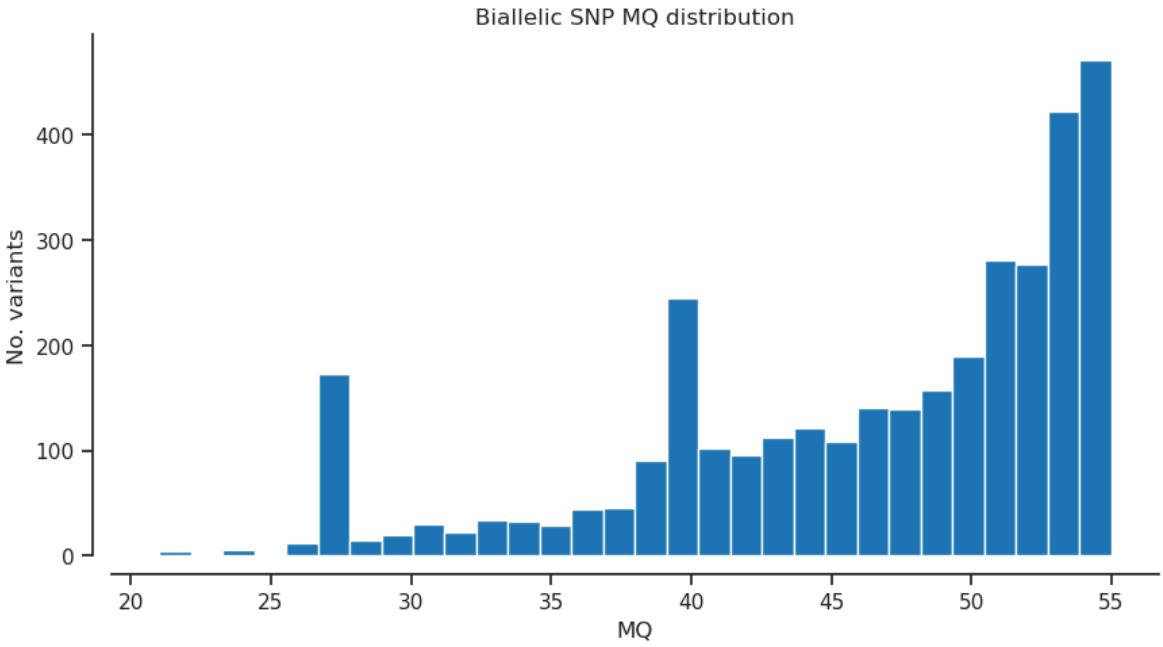


In [15]:
```
plot_hist('MQ','biallelic') # RMS mapping quality
```



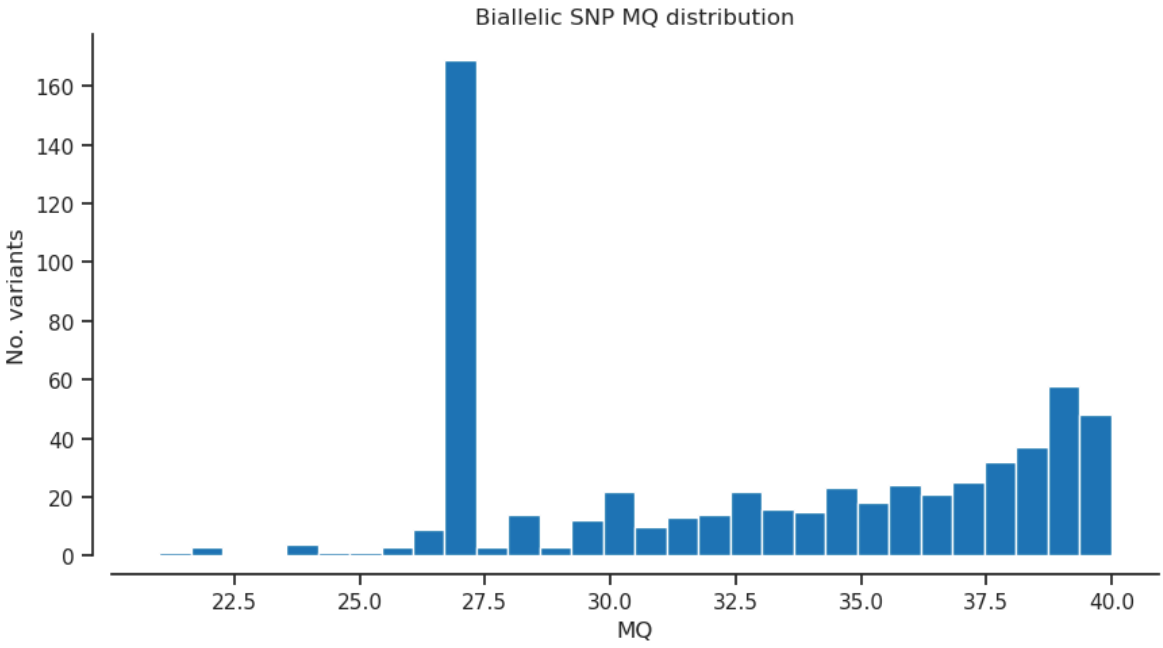
In [16]:
```
filter_expression = '(MQ < 55)'
bi_selection = biallelic_np.query(filter_expression)[:]
#np.count_nonzero(var_selection)
```

In [17]:
```
plot_hist('MQ')
```

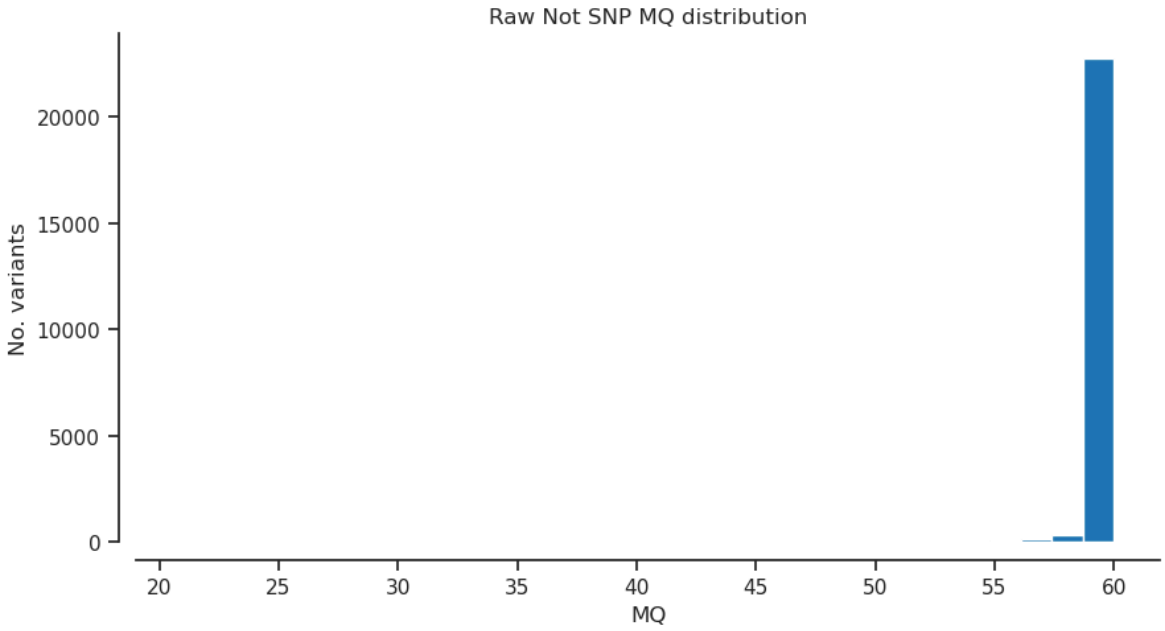


In [18]:
```
filter_expression = '(MQ < 40)'
bi_selection = biallelic_np.query(filter_expression)[:]
```

In [19]:
```
plot_hist('MQ')
```

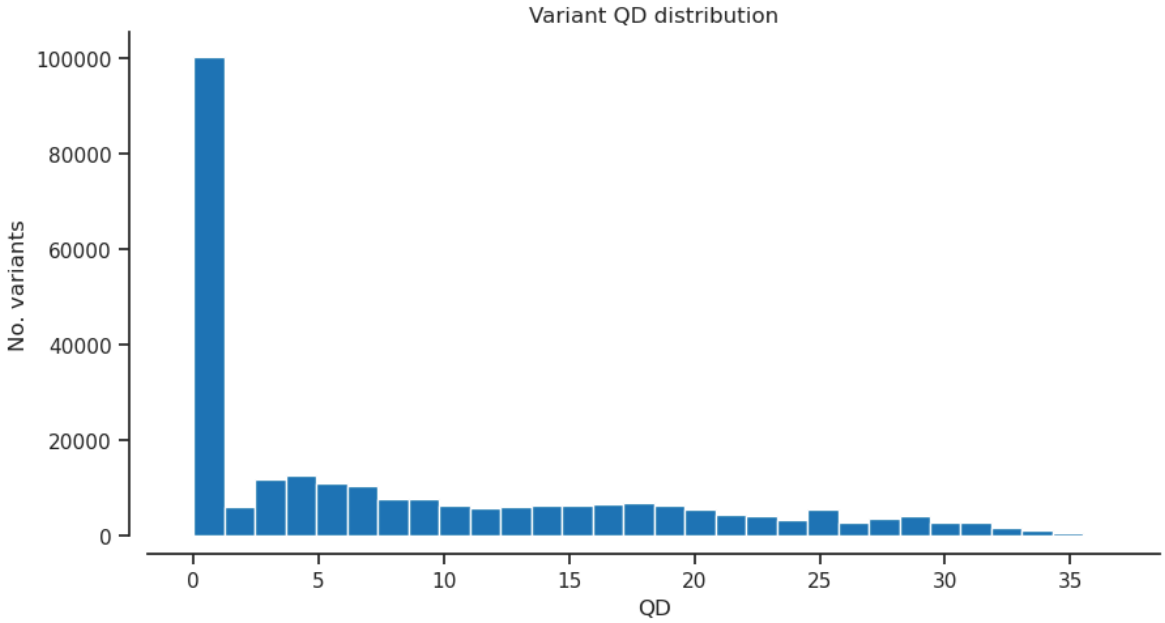


In [20]:
```
plot_hist('MQ','notsnp')
```

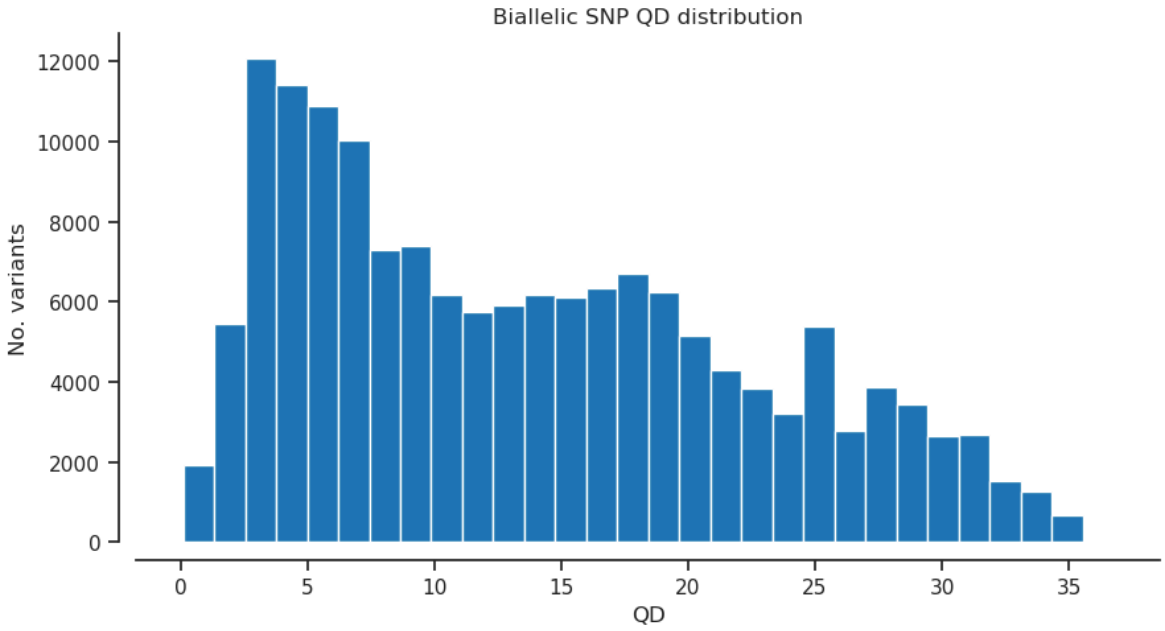


QD - Variant Confidence/Quality by Depth

In [21]:
```
plot_hist('QD','var') # Variant Confidence/Quality by Depth
```

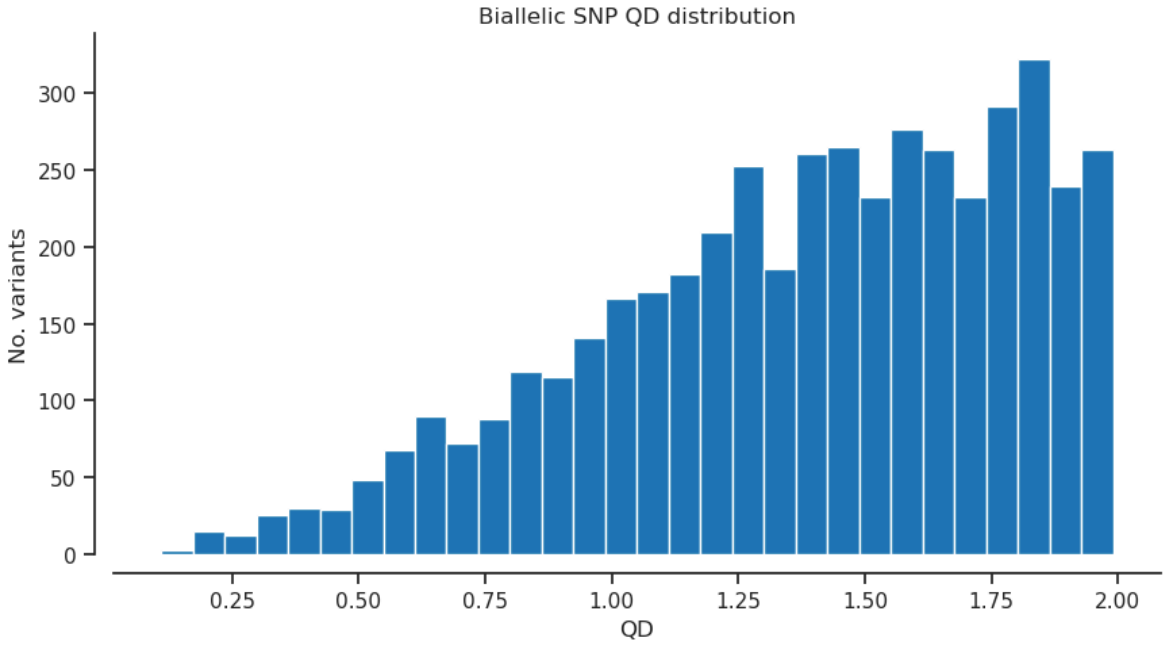


In [22]:
```
plot_hist('QD','biallelic') # Variant Confidence/Quality by Depth
```

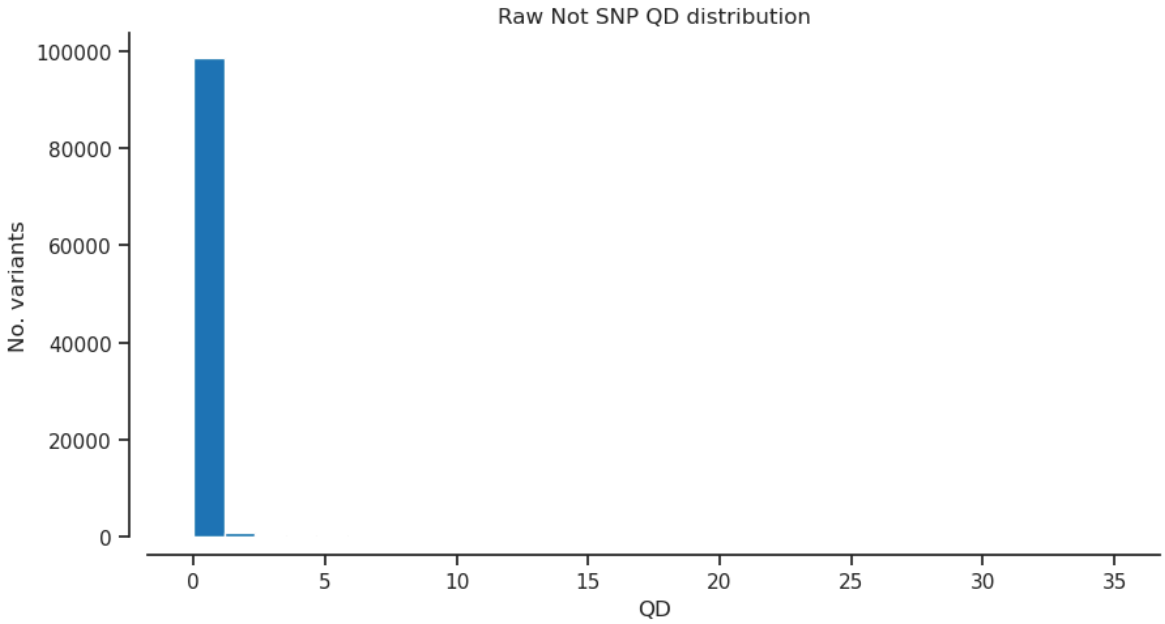


In [23]:
```
filter_expression = '(QD < 2)'
bi_selection = biallelic_np.query(filter_expression)[:]
```

In [24]:
```
plot_hist('QD')
```

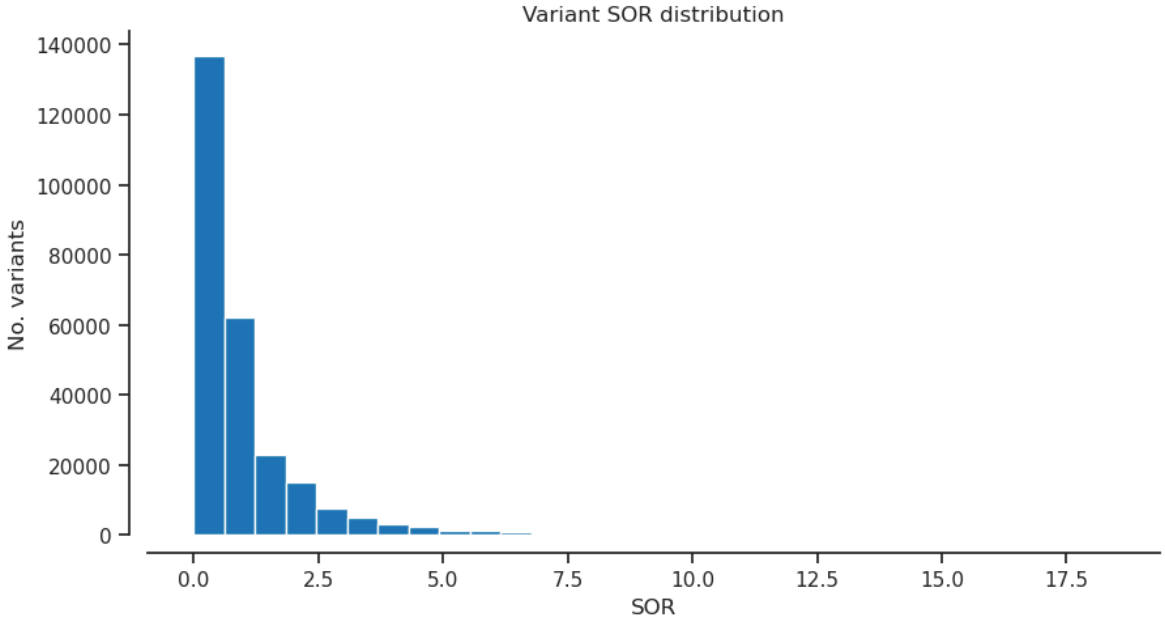


In [25]:
```
plot_hist('QD','notsnp') # Variant Confidence/Quality by Depth
```

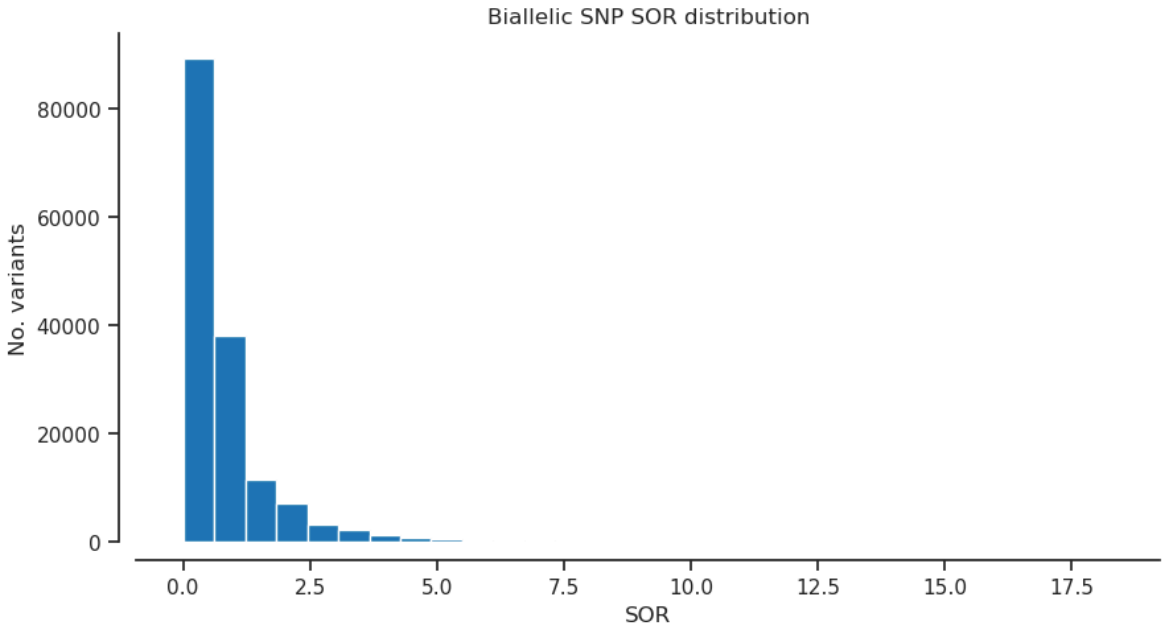


SOR - Symmetric Odds Ratio of 2x2 contingency table to detect strand bias

In [26]:
```
plot_hist('SOR', 'var') # Symmetric Odds Ratio of 2x2 contingency table t
```

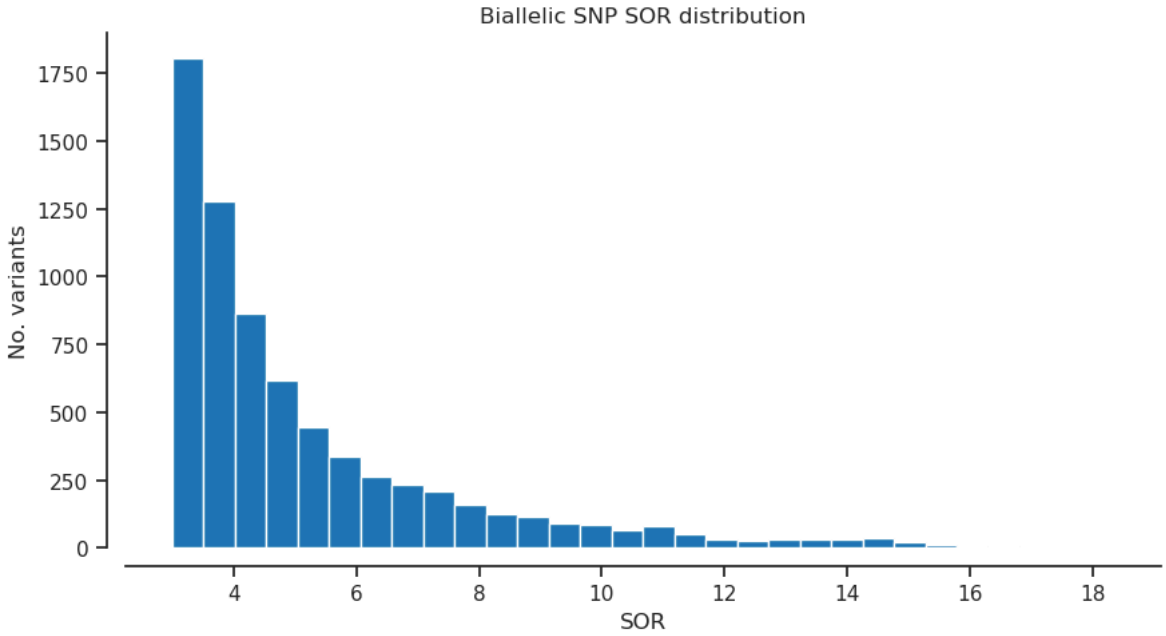


In [27]:
```
plot_hist('SOR','biallelic') # Symmetric Odds Ratio of 2x2 contingency ta
```

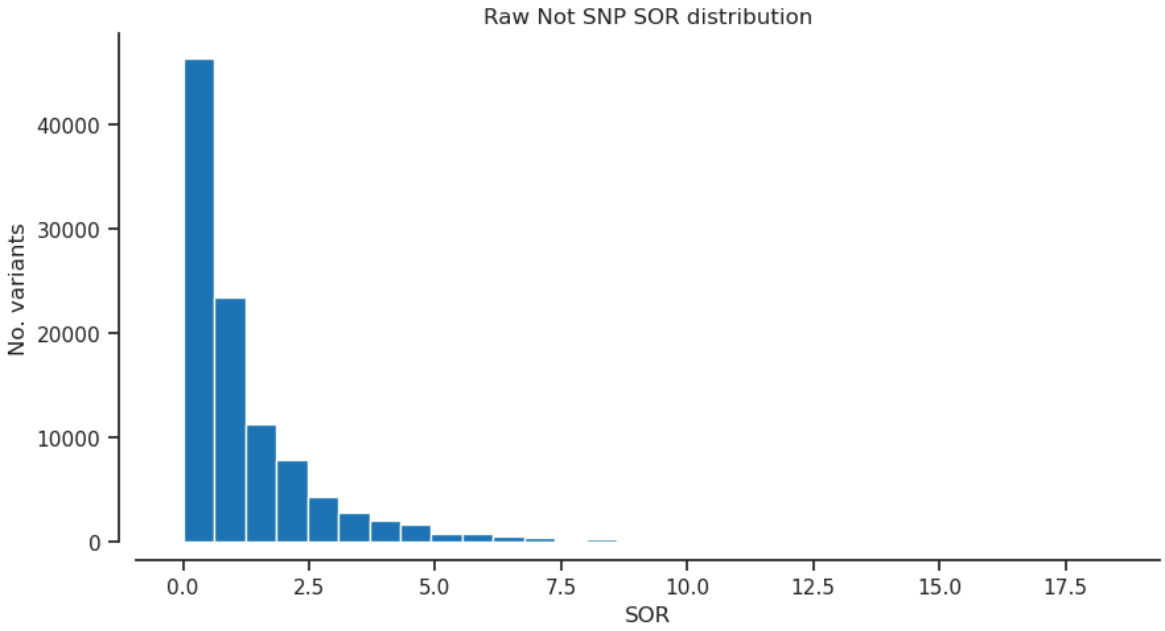


In [28]:
```
filter_expression = '(SOR > 3)'
bi_selection = biallelic_np.query(filter_expression)[:]
```

In [29]:
```
plot_hist('SOR') # Symmetric Odds Ratio of 2x2 contingency table to detec
```

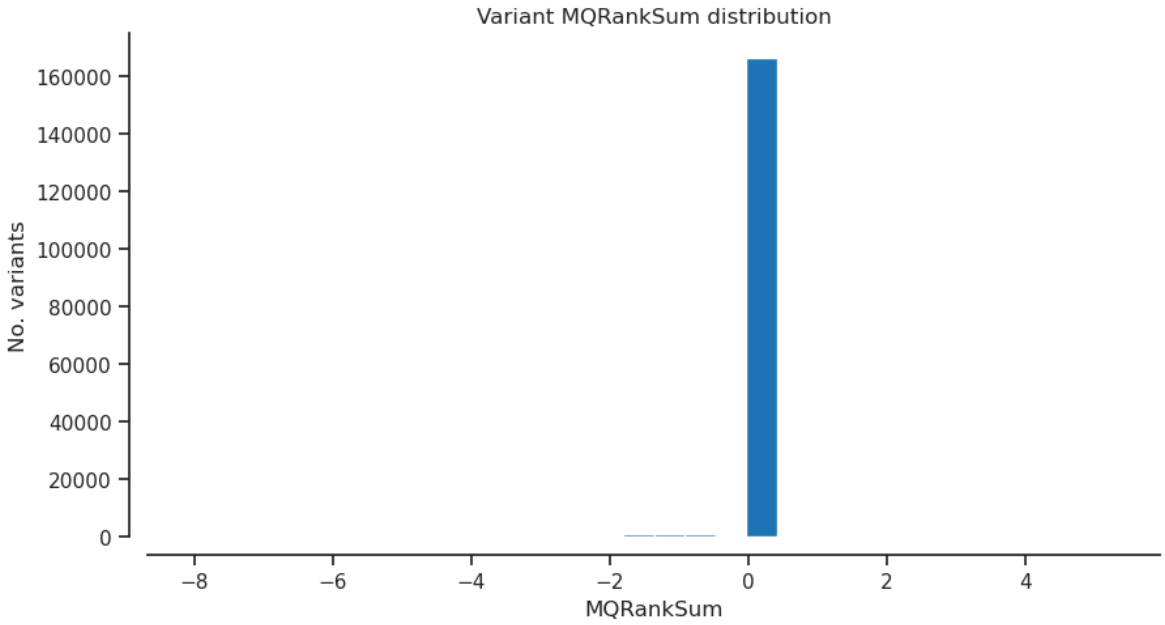


In [30]:
```
plot_hist('SOR','notsnp') # Symmetric Odds Ratio of 2x2 contingency table
```

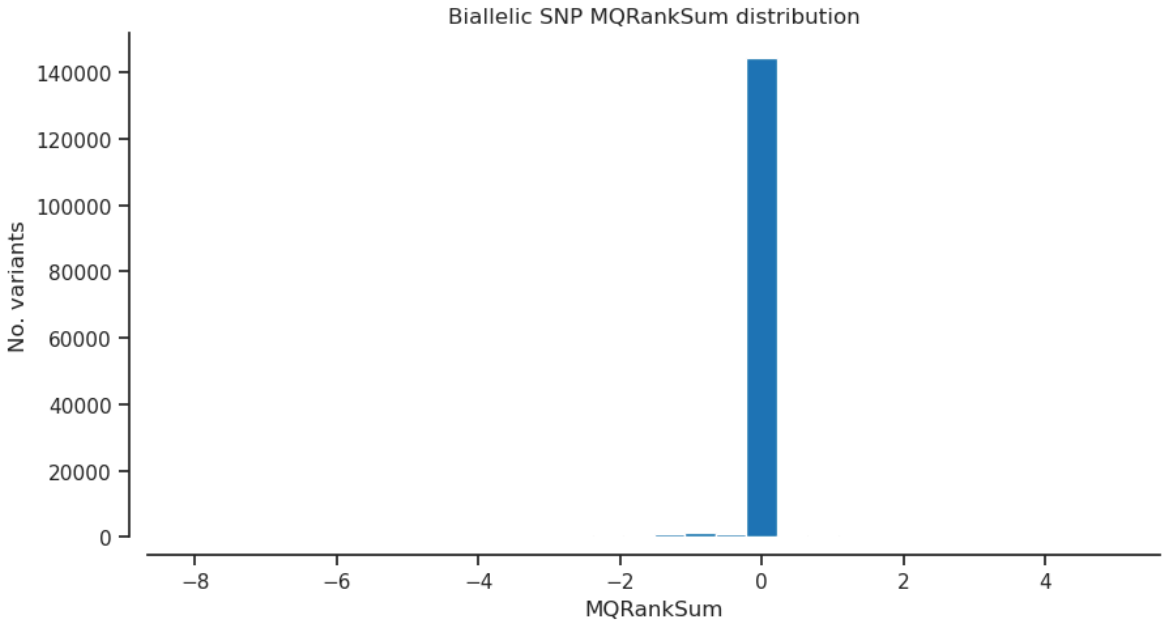


MQRankSum - Z-score From Wilcoxon rank sum test of Alt vs. Ref read mapping qualities

In [31]:
```
plot_hist('MQRankSum','var') # Z-score From Wilcoxon rank sum test of Alt
```

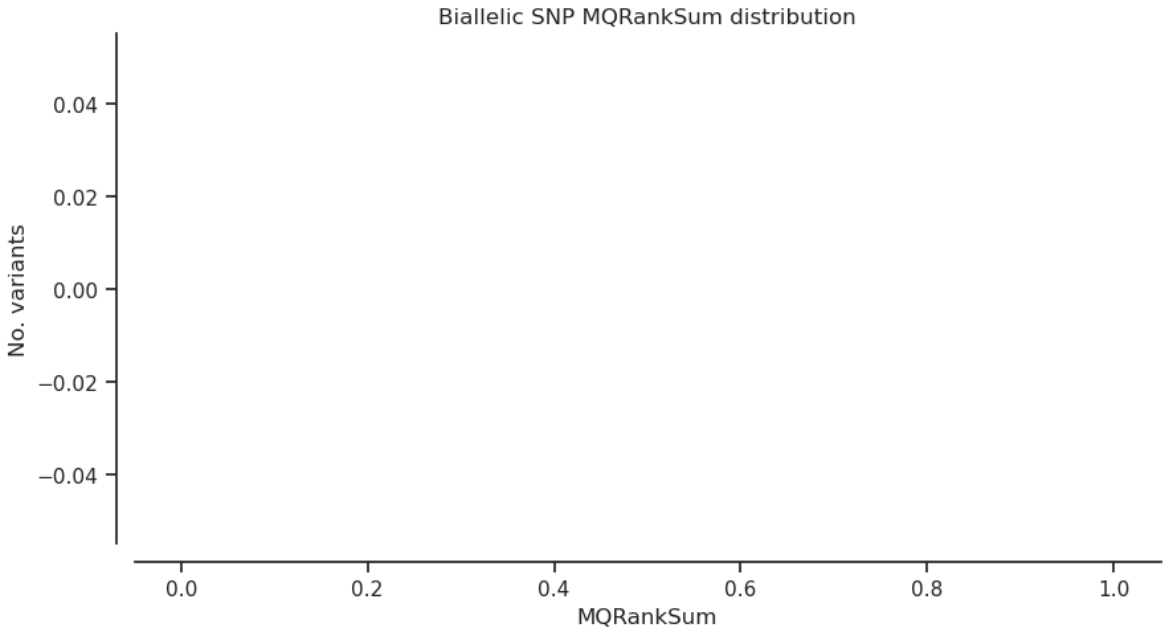


In [32]:
```
plot_hist('MQRankSum','biallelic') # Z-score From Wilcoxon rank sum test
```

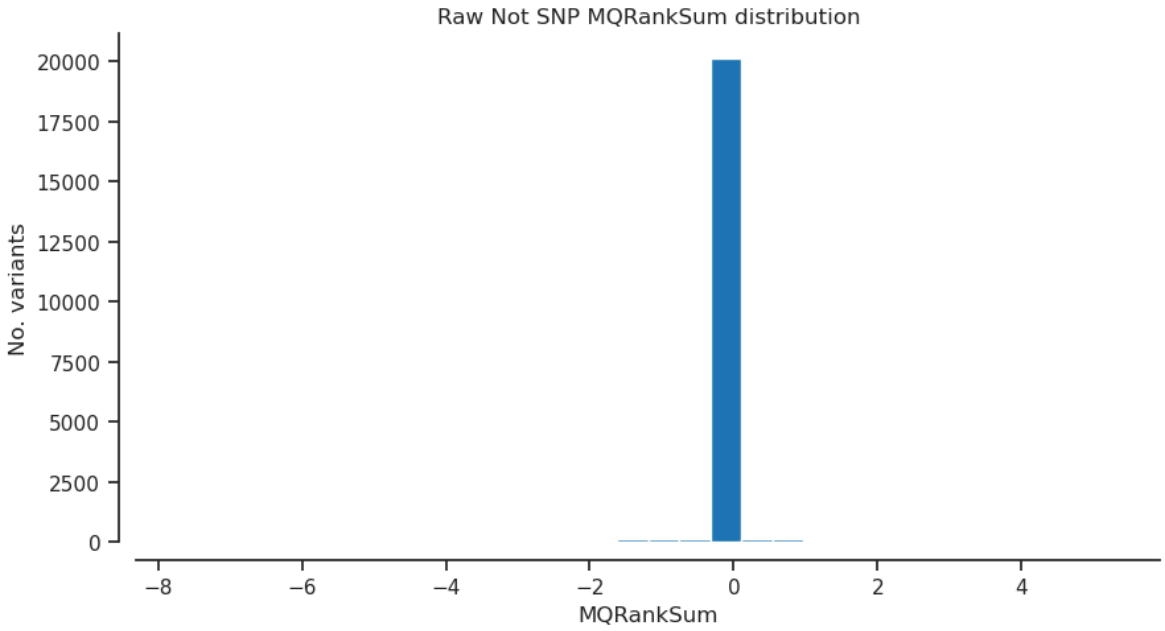


In [33]:
```
filter_expression = '(MQRankSum < -12.5)'
bi_selection = biallelic_np.query(filter_expression)[:]
```

In [34]:
```
plot_hist('MQRankSum') # Z-score From Wilcoxon rank sum test of Alt vs. R
```

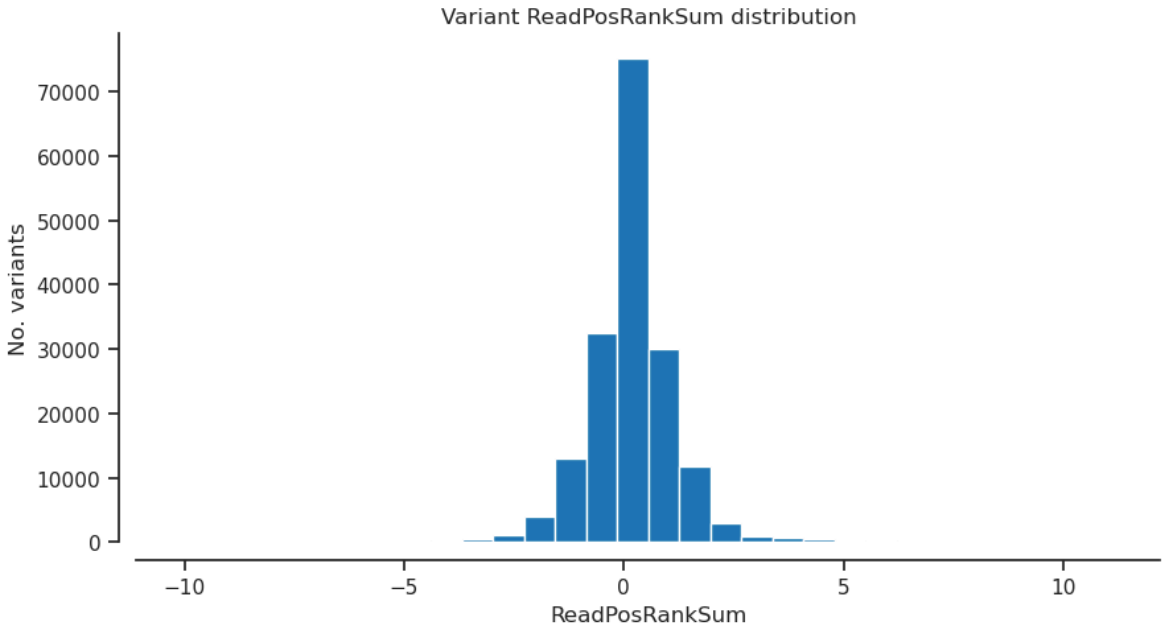


In [35]:
```
plot_hist('MQRankSum','notsnp') # Z-score From Wilcoxon rank sum test of
```

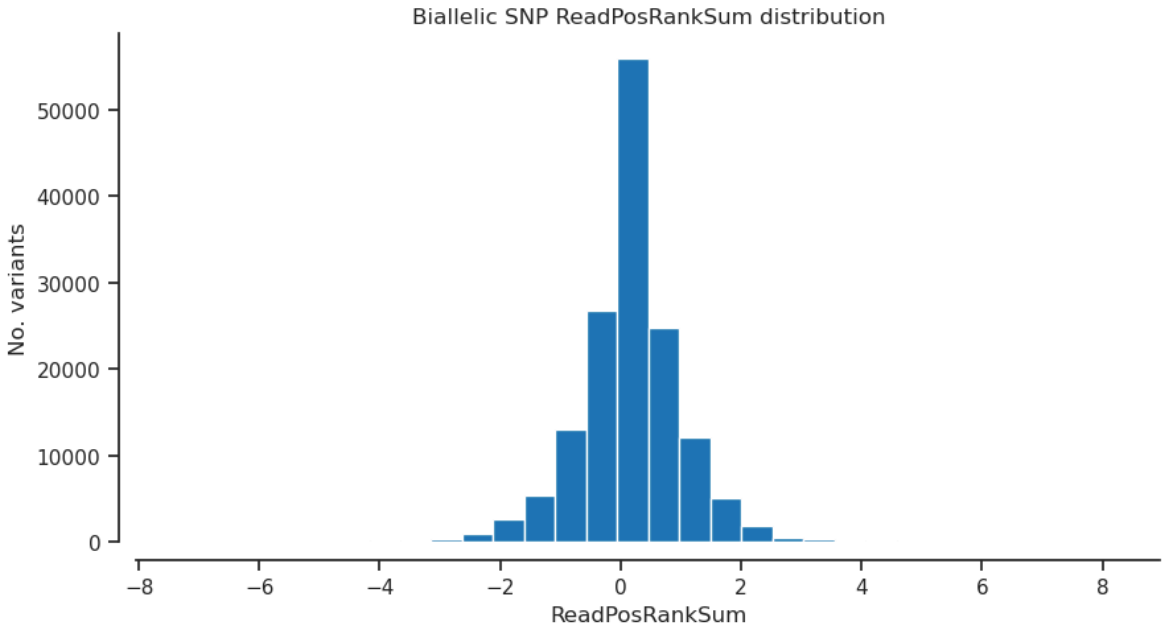


ReadPosRankSum - Z-score from Wilcoxon rank sum test of Alt vs. Ref read position bias

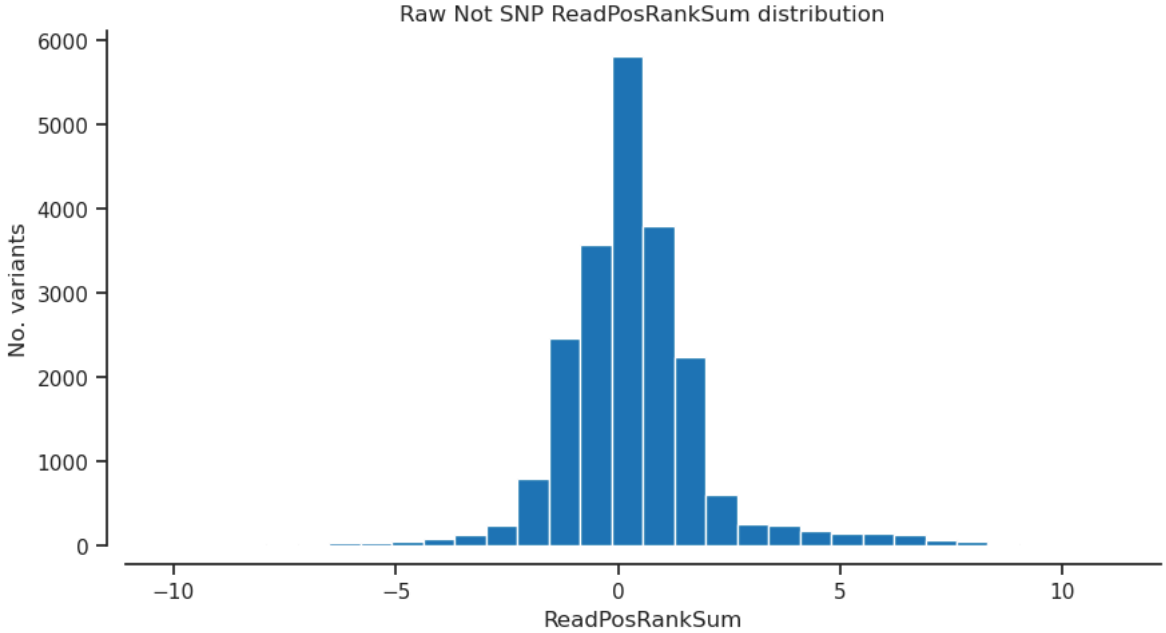
In [36]:
```
plot_hist('ReadPosRankSum','var') # Z-score from Wilcoxon rank sum test o
```



In [37]:
```
plot_hist('ReadPosRankSum','biallelic') # Z-score from Wilcoxon rank sum
```

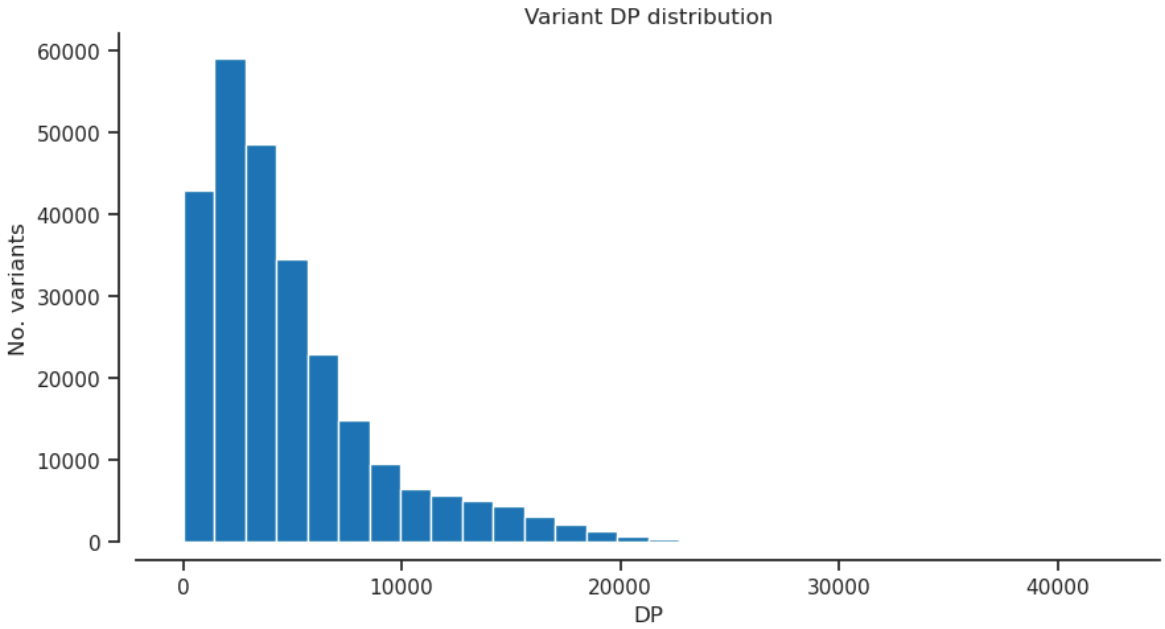


In [38]:
```
plot_hist('ReadPosRankSum','notsnp') # Z-score from Wilcoxon rank sum tes
```

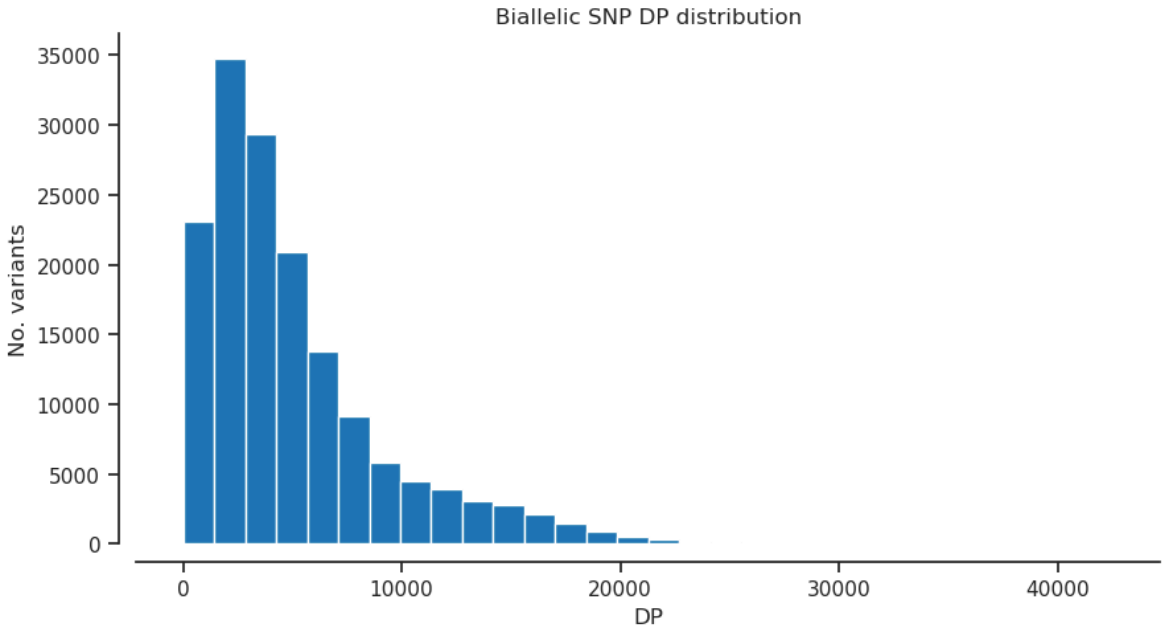


DP - Approximate read depth

In [39]:
```
plot_hist('DP','var')
```

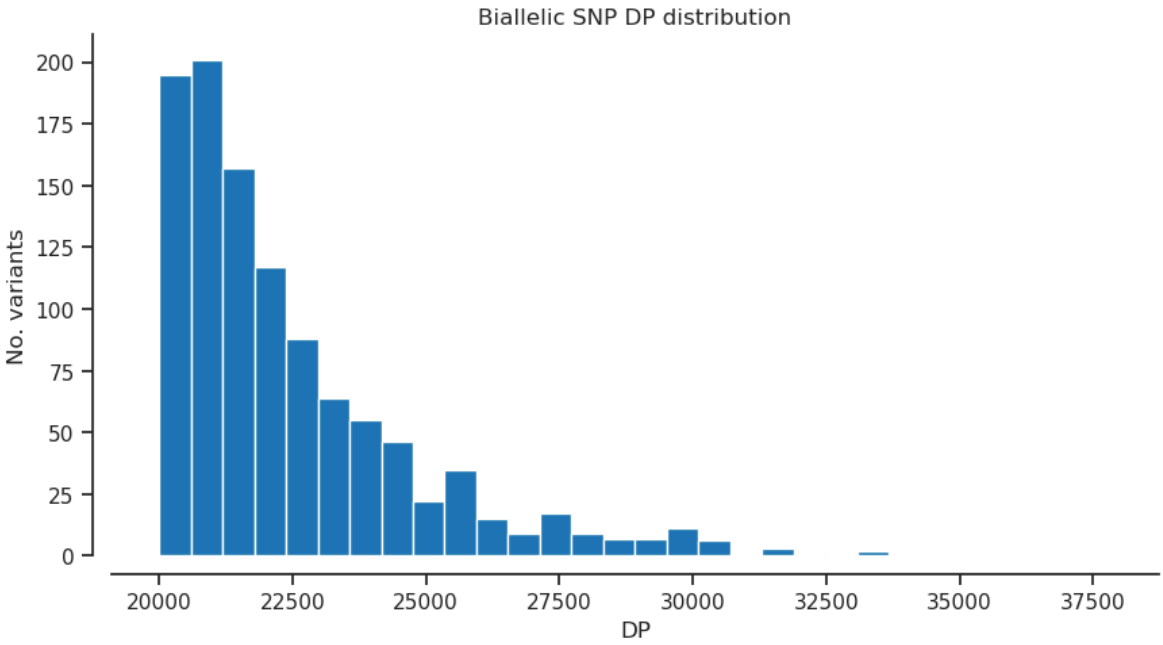


In [40]:
```
plot_hist('DP','biallelic')
```

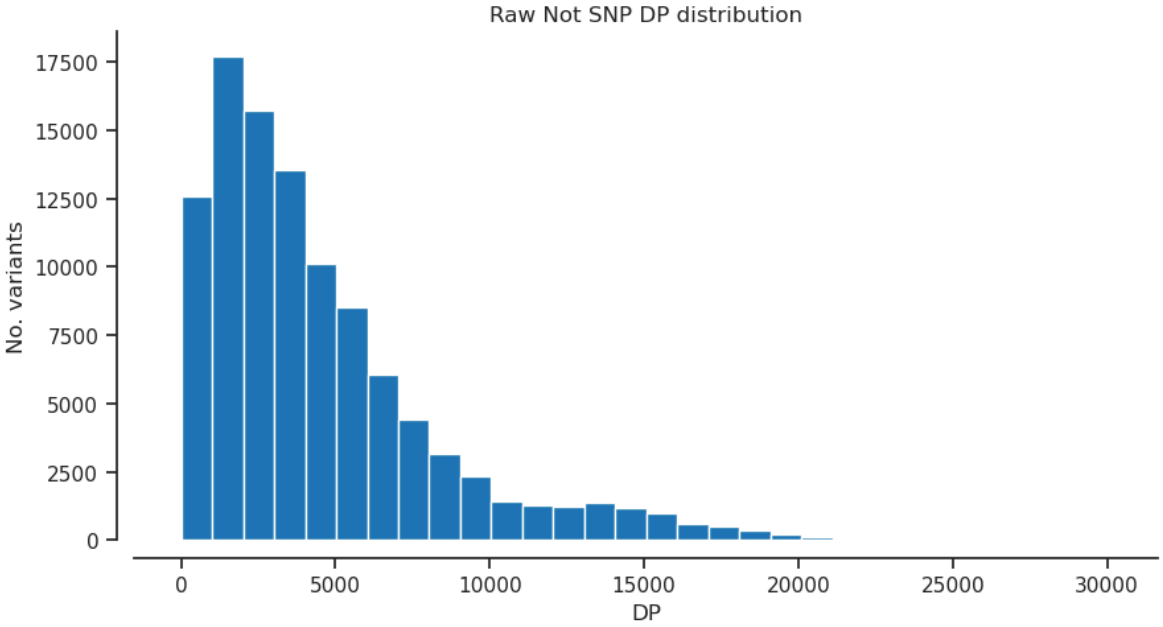


In [41]:
```
filter_expression = '(DP > 20000) & (DP < 40000)'
bi_selection = biallelic_np.query(filter_expression)[:]
```

In [42]:
```
plot_hist('DP')
```

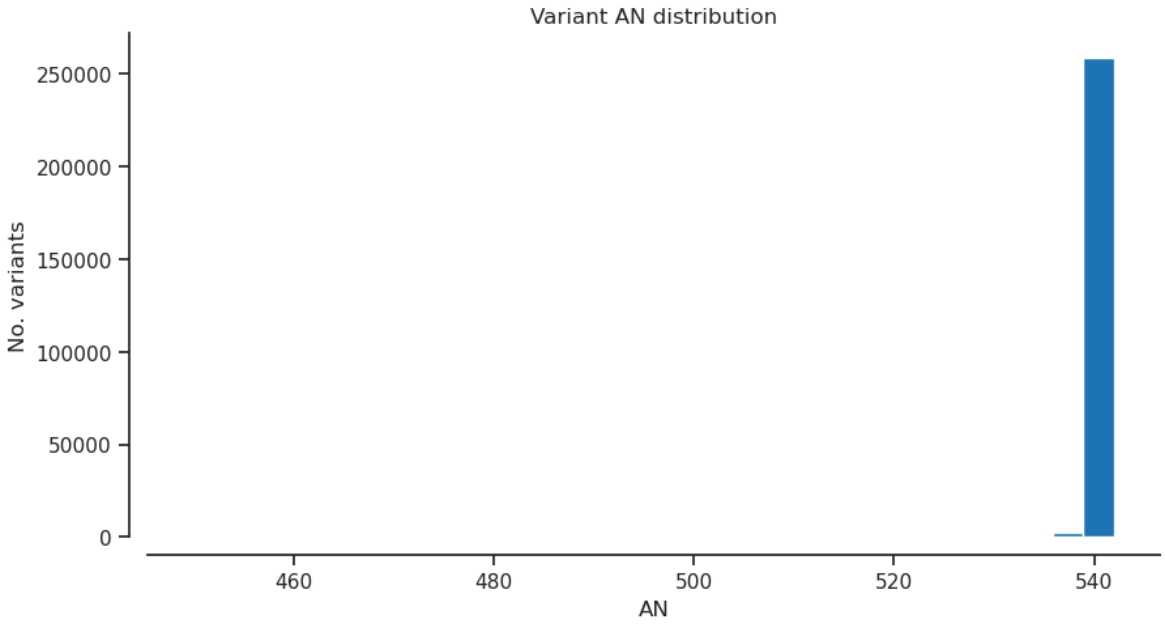


In [43]:
```
plot_hist('DP','notsnp')
```

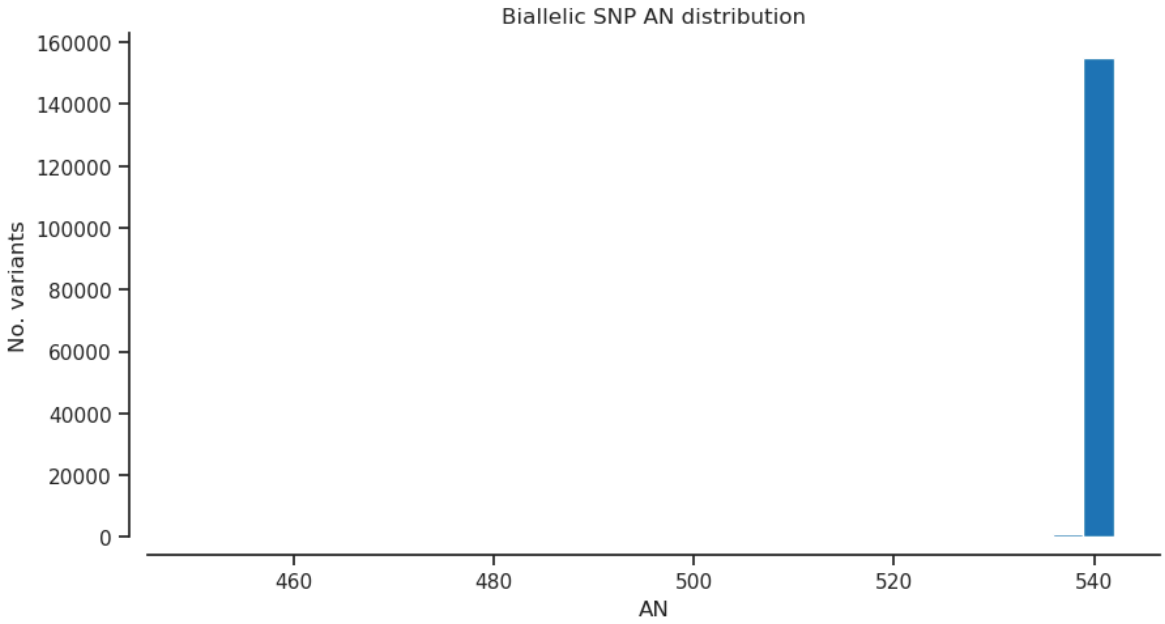


AN - Total number of alleles in called genotypes

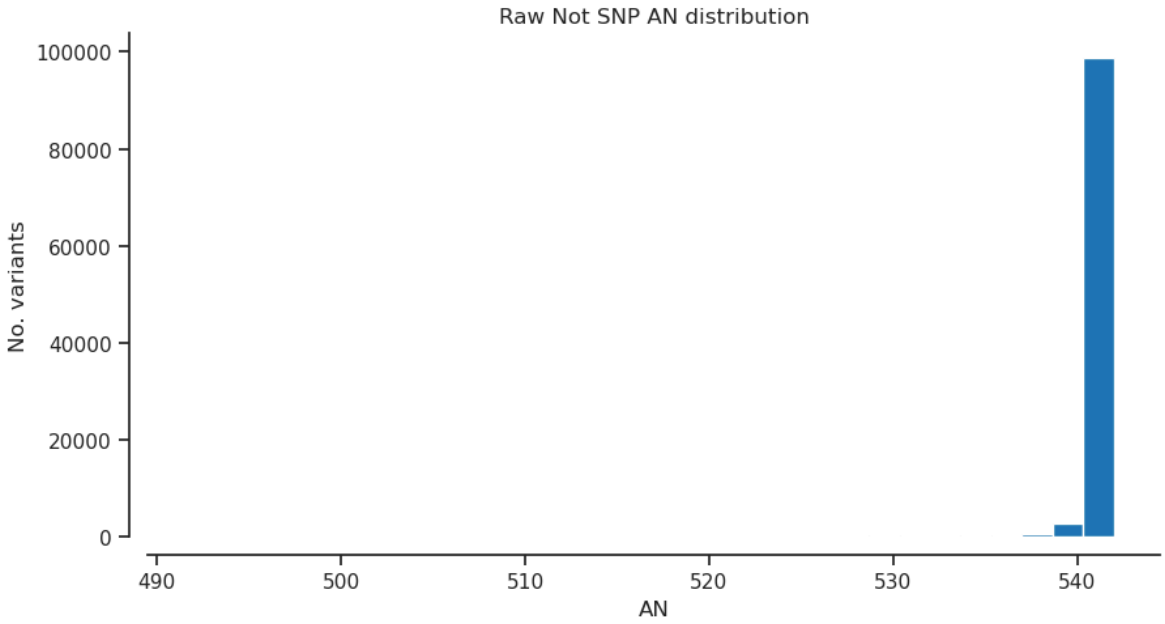
In [44]:
```
plot_hist('AN','var') # Total number of alleles in called genotypes
```



In [45]:
```
plot_hist('AN','biallelic') # Total number of alleles in called genotypes
```



In [46]:
```
plot_hist('AN','notsnp') # Total number of alleles in called genotypes
```



Selected filter

In [47]:
```
# QD: Variant Confidence/Quality by Depth
# AN: Total number of alleles in called genotypes
filter_expression = '(QD >= 2) & (MQ >= 40) & (MQRankSum >= -12.5) & (is_
variant_selection = variants_np.eval(filter_expression)[:]
np.count_nonzero(variant_selection)
```

Out[47]:
```
148083
```

Genotype

In [48]:
```
calldata_var = callset_var['calldata']
list(calldata_var)
```

Out[48]:
```
['AD', 'DP', 'GQ', 'GT', 'MIN_DP', 'PGT', 'PID', 'PL', 'PS', 'RGQ', 'S
B']
```

In [49]:
```
genotypes_var = allel.GenotypeChunkedArray(calldata_var['GT'])
genotypes_var
```

Out[49]: <GenotypeChunkedArray shape=(262360, 271, 2) dtype=int8 chunks=(65536, 64, 2) nbytes=135.6M cbytes=5.8M cratio=23.2 compression=gzip compression_opts=1 values=h5py._hl.dataset.Dataset>

	0	1	2	3	4	...	266	267	268	269	270
0	0/0	0/0	0/0	0/0	0/0	...	0/0	0/0	0/0	0/0	0/0
1	0/0	0/0	0/0	0/0	0/0	...	0/0	0/0	0/0	0/0	0/0
2	0/0	0/0	0/0	0/0	0/0	...	0/0	0/0	0/0	0/0	0/0
...						...					
262357	0/0	0/0	0/0	0/0	0/0	...	0/0	0/0	0/0	0/0	0/0
262358	0/0	0/0	0/0	0/0	0/0	...	0/0	0/0	0/0	0/0	0/0
262359	0/0	0/0	0/0	0/0	0/0	...	0/0	0/0	0/0	0/0	0/0

In [50]:
```
# using the selected filters set above
gt_filtered_snps = genotypes_var.subset(variant_selection)
gt_filtered_snps
```

Out[50]: <GenotypeChunkedArray shape=(148083, 271, 2) dtype=int8 chunks=(2314, 271, 2) nbytes=76.5M cbytes=6.1M cratio=12.5 compression=blosc compression_opts={'cname': 'lz4', 'clevel': 5, 'shuffle': 1, 'blocksize': 0} values=zarr.core.Array>

	0	1	2	3	4	...	266	267	268	269	270
0	0/0	0/0	0/0	0/0	0/0	...	0/0	0/0	0/0	0/0	0/0
1	0/0	0/0	0/0	0/0	0/0	...	0/0	0/0	0/0	0/0	0/0
2	0/0	0/0	0/0	0/0	0/0	...	0/0	0/0	0/0	0/0	0/0
...						...					
148080	0/0	0/0	0/0	0/0	0/0	...	0/0	0/0	0/0	0/0	0/0
148081	0/0	0/0	0/0	0/0	0/0	...	0/0	0/0	0/0	0/0	0/0
148082	0/0	0/0	0/0	0/0	0/0	...	0/0	0/0	0/0	0/0	0/0

In [51]:
```
# grab the allele counts for the populations
ac = gt_filtered_snps.count_alleles()
ac
```

Out[51]: <AlleleCountsChunkedArray shape=(148083, 4) dtype=int32 chunks=(18511, 4) nbytes=2.3M cbytes=381.2K cratio=6.1 compression=blosc compression_opts={'cname': 'lz4', 'clevel': 5, 'shuffle': 1, 'blocksize': 0} values=zarr.core.Array>

	0	1	2	3
0	538	4	0	0
1	538	4	0	0
2	541	1	0	0
...		...		
148080	540	2	0	0
148081	541	1	0	0
148082	541	1	0	0

In [52]:
```
ac[:]
```

Out[52]: <AlleleCountsArray shape=(148083, 4) dtype=int32>

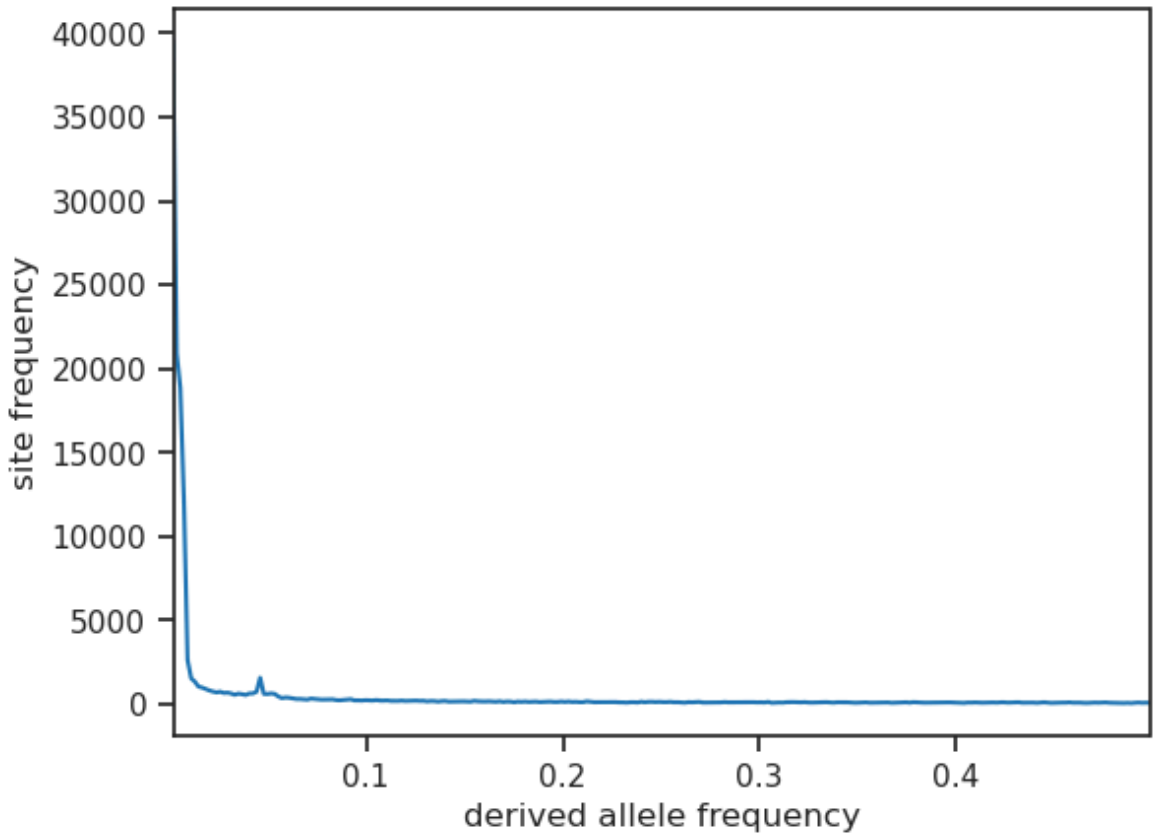
	0	1	2	3
0	538	4	0	0
1	538	4	0	0
2	541	1	0	0
...		...		
148080	540	2	0	0
148081	541	1	0	0
148082	541	1	0	0

In [53]:
```
# Which ones are biallelic?
is_biallelic_01 = ac.is_biallelic_01()[:]
ac1 = ac.compress(is_biallelic_01, axis=0)[:, :2]
ac1
##this part of the code is only for graphing the SFS, is not useful for f
```

Out[53]:
```
array([[538,   4],
       [538,   4],
       [541,   1],
       ...,
       [540,   2],
       [541,   1],
       [541,   1]], dtype=int32)
```

In [54]:
```
# plot the sfs of the derived allele
s = allel.sfs_folded(ac1)
allel.plot_sfs(s, yscale="linear", n=ac1.sum(axis=1).max())
```

Out[54]:
```
<Axes: xlabel='derived allele frequency', ylabel='site frequency'>
```



In [55]:
```
biallelic = (ac.max_allele() == 1)
###This is the filter expression for biallelic sites
biallelic
```

Out[55]:
```
<ChunkedArrayWrapper shape=(148083,) dtype=bool chunks=(148083,)
   nbytes=144.6K cbytes=10.2K cratio=14.2
   compression=blosc compression_opts={'cname': 'lz4', 'clevel': 5, 'shu
ffle': 1, 'blocksize': 0}
   values=zarr.core.Array>
```

In [56]:
```
# select only the biallelic variants
gt_biallelic = gt_filtered_snps.compress(biallelic)
gt_biallelic
```

Out[56]:
<GenotypeChunkedArray shape=(146128, 271, 2) dtype=int8 chunks=(2284, 271, 2) nbytes=75.5M cbytes=6.0M cratio=12.5 compression=blosc compression_opts={'cname': 'lz4', 'clevel': 5, 'shuffle': 1, 'blocksize': 0} values=zarr.core.Array>

	0	1	2	3	4	...	266	267	268	269	270
0	0/0	0/0	0/0	0/0	0/0	...	0/0	0/0	0/0	0/0	0/0
1	0/0	0/0	0/0	0/0	0/0	...	0/0	0/0	0/0	0/0	0/0
2	0/0	0/0	0/0	0/0	0/0	...	0/0	0/0	0/0	0/0	0/0
...						...					
146125	0/0	0/0	0/0	0/0	0/0	...	0/0	0/0	0/0	0/0	0/0
146126	0/0	0/0	0/0	0/0	0/0	...	0/0	0/0	0/0	0/0	0/0
146127	0/0	0/0	0/0	0/0	0/0	...	0/0	0/0	0/0	0/0	0/0

In [57]:
```
n_variants = len(gt_biallelic)
n_variants
```

Out[57]: 146128

In [58]:
```
pc_missing = gt_biallelic.count_missing(axis=0)[:] * 100 / n_variants
pc_het = gt_biallelic.count_het(axis=0)[:] * 100 / n_variants
```

Samples

In [59]:
```
samples_var = callset_var['samples']
samples_var = list(samples_var)
samples_var
```

Out[59]:
```
[b'BEL00006-001',
 b'BEL00006-002',
 b'BEL00006-003',
 b'BEL00006-004',
 b'BEL00006-005',
 b'BEL00006-006',
 b'BEL00006-007',
 b'BEL00006-008',
 b'BEL00006-009',
 b'BEL00006-010',
 b'BEL00006-011',
 b'BEL00006-012',
 b'BEL00006-013',
 b'BEL00006-014',
 b'BEL00006-015',
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 b'BEL00006-017',
 b'BEL00006-018',
 b'BEL00006-019',
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 b'BEL00006-022',
 b'BEL00006-023',
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 b'BEL00007-003',
 b'BEL00007-004',
 b'BEL00007-005',
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 b'BEL00007-007',
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 b'BEL00007-018',
 b'BEL00007-019',
 b'BEL00007-020',
 b'BEL00007-021',
 b'BEL00007-022',
 b'BEL00007-023',
 b'BEL00007-024',
 b'BEL00007-025',
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 b'BGR00002-003',
 b'BGR00002-004',
 b'BGR00002-005',
 b'BGR00002-006',
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 b'BGR00002-008',
 b'BGR00002-009',
 b'BGR00002-010',
```

```
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b'BGR00002-014',
b'BGR00002-015',
b'BGR00002-016',
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b'BGR00002-021',
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b'BGR00002-024',
b'BGR00002-025',
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b'CZE00156-003',
b'CZE00156-004',
b'CZE00156-005',
b'CZE00156-006',
b'CZE00156-007',
b'CZE00156-008',
b'CZE00156-009',
b'CZE00156-010',
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b'CZE00156-016',
b'CZE00156-017',
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b'CZE00156-021',
b'CZE00156-022',
b'CZE00156-023',
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b'DEU00001-015',
b'DEU00001-016',
b'DEU00001-017',
b'DEU00001-018',
b'DEU00001-019',
b'DEU00001-020',
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```
b'DEU00001-021',
b'DEU00001-022',
b'DEU00001-023',
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b'ESP00082-001',
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b'TUR00228-012',
b'TUR00228-013',
b'TUR00228-014',
b'TUR00228-015',
```

```
 b'TUR00228-016',
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 b'TUR00228-018',
 b'TUR00228-019',
 b'TUR00228-020',
 b'TUR00228-021',
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 b'TUR00231-004',
 b'TUR00231-005',
 b'TUR00231-006',
 b'TUR00231-007',
 b'TUR00231-008',
 b'TUR00231-009',
 b'TUR00231-010',
 b'TUR00231-011',
 b'TUR00231-012']
```

In [62]:
```
samples_fn = '~/scratch/data/Pavium/Prunus_avium_sample_list_scikit-allel
samples = pandas.read_csv(samples_fn, sep='\t')
samples
```

Out[62]:

	ID	Population
0	BEL00006-001	BEL00006
1	BEL00006-002	BEL00006
2	BEL00006-003	BEL00006
3	BEL00006-004	BEL00006
4	BEL00006-005	BEL00006
...	...	...
266	TUR00231-008	TUR00231
267	TUR00231-009	TUR00231
268	TUR00231-010	TUR00231
269	TUR00231-011	TUR00231
270	TUR00231-012	TUR00231

271 rows × 2 columns

In [63]:
```
samples.Population.value_counts()
```

Out[63]:
```
Population
BEL00006    25
BEL00007    25
BGR00002    25
CZE00156    25
DEU00001    25
ESP00082    25
ESP00219    25
ESP00246    25
NLD00003    25
TUR00228    22
TUR00231    12
TUR00229     8
TUR00230     4
Name: count, dtype: int64
```

In [64]:
```
populations = samples.Population.unique()
populations
###This identifiers come from the metadata file
```

Out[64]:
```
array(['BEL00006', 'BEL00007', 'BGR00002', 'CZE00156', 'DEU00001',
       'ESP00082', 'ESP00219', 'ESP00246', 'NLD00003', 'TUR00228',
       'TUR00229', 'TUR00230', 'TUR00231'], dtype=object)
```

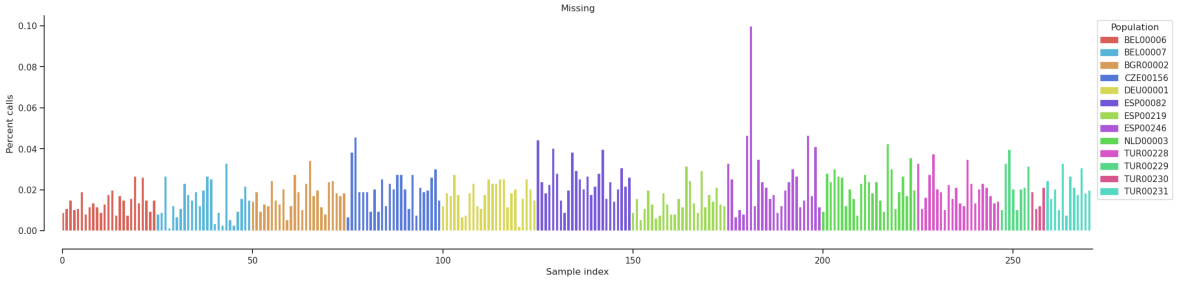
Gt frequency function

In [71]:
```
def plot_genotype_frequency(pc, title):
    fig, ax = plt.subplots(figsize=(24, 5))
    sns.despine(ax=ax, offset=24)
    left = np.arange(len(pc))
    palette = sns.color_palette("hls", 13)
    pop2color = {'BEL00006': palette[0],
                 'BEL00007': palette[7],
                 'BGR00002': palette[1],
                 'CZE00156': palette[8],
                 'DEU00001': palette[2],
                 'ESP00082': palette[9],
                 'ESP00219': palette[3],
                 'ESP00246': palette[10],
                 'NLD00003': palette[4],
                 'TUR00228': palette[11],
                 'TUR00229': palette[5],
                 'TUR00230': palette[12],
                 'TUR00231': palette[6]}
    colors = [pop2color[p] for p in samples.Population]
    ax.bar(left, pc, color=colors)
    ax.set_xlim(0, len(pc))
    ax.set_xlabel('Sample index')
    ax.set_ylabel('Percent calls')
    ax.set_title(title)
    handles = [mpl.patches.Patch(color=palette[0]),
               mpl.patches.Patch(color=palette[7]),
               mpl.patches.Patch(color=palette[1]),
               mpl.patches.Patch(color=palette[8]),
               mpl.patches.Patch(color=palette[2]),
               mpl.patches.Patch(color=palette[9]),
```

```
                mpl.patches.Patch(color=palette[3]),
                mpl.patches.Patch(color=palette[10]),
                mpl.patches.Patch(color=palette[4]),
                mpl.patches.Patch(color=palette[11]),
                mpl.patches.Patch(color=palette[5]),
                mpl.patches.Patch(color=palette[12]),
                mpl.patches.Patch(color=palette[6])]
    ax.legend(handles=handles, labels=['BEL00006', 'BEL00007', 'BGR00002'
       'ESP00082', 'ESP00219', 'ESP00246', 'NLD00003', 'TUR00228', 'TUR00
       'TUR00230', 'TUR00231'], title='Population',
              bbox_to_anchor=(1, 1), loc='upper left')
```

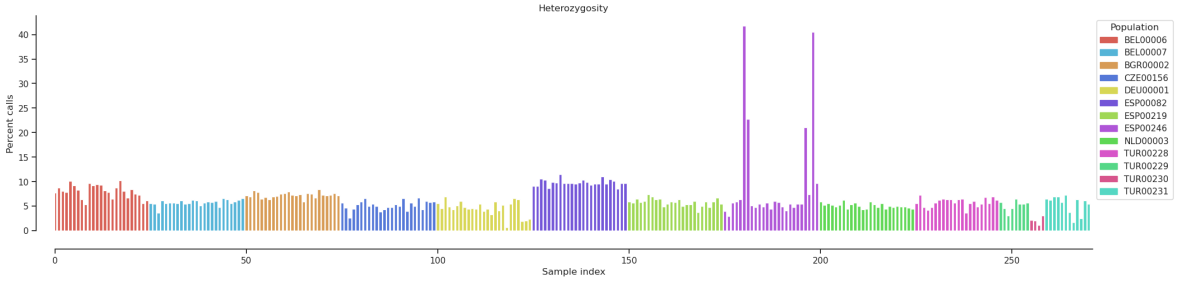
Plot missing

In [72]:
```
plot_genotype_frequency(pc_missing, 'Missing')
```



Plot heterozygosity

In [73]:
```
plot_genotype_frequency(pc_het, 'Heterozygosity')
```



PCA

In [74]:
```
palette = sns.color_palette("hls",13)
pop_colours = {
                'BEL00006': palette[0],
                 'BEL00007': palette[7],
                 'BGR00002': palette[1],
                 'CZE00156': palette[8],
                 'DEU00001': palette[2],
                 'ESP00082': palette[9],
                 'ESP00219': palette[3],
                 'ESP00246': palette[10],
                 'NLD00003': palette[4],
                 'TUR00228': palette[11],
                 'TUR00229': palette[5],
                 'TUR00230': palette[12],
```

```
                'TUR00231': palette[6]
}
```

In [75]:
```
def plot_pca_coords(coords, model, pc1, pc2, ax, sample_population):
    sns.despine(ax=ax, offset=5)
    x = coords[:, pc1]
    y = coords[:, pc2]
    for pop in populations:
        flt = (sample_population == pop)
        ax.plot(x[flt], y[flt], marker='o', linestyle=' ', color=pop_colo
                label=pop, markersize=6, mec='k', mew=.5)
    ax.set_xlabel('PC%s (%.1f%%)' % (pc1+1, model.explained_variance_rati
    ax.set_ylabel('PC%s (%.1f%%)' % (pc2+1, model.explained_variance_rati


def fig_pca(coords, model, title, sample_population=None):
    if sample_population is None:
        sample_population = samples.Population
    # plot coords for PCs 1 vs 2, 3 vs 4
    fig = plt.figure(figsize=(10, 5))
    ax = fig.add_subplot(1, 2, 1)
    plot_pca_coords(coords, model, 0, 1, ax, sample_population)
    ax = fig.add_subplot(1, 2, 2)
    plot_pca_coords(coords, model, 2, 3, ax, sample_population)
    ax.legend(bbox_to_anchor=(1, 1), loc='upper left')
    fig.suptitle(title, y=1.02)
    fig.tight_layout()
```

In [76]:
```
ac2 = gt_biallelic.count_alleles()
ac2
```

Out[76]:
<AlleleCountsChunkedArray shape=(146128, 2) dtype=int32 chunks=(36532, 2) nbytes=1.1M cbytes=294.8K cratio=3.9 compression=blosc compression_opts={'cname': 'lz4', 'clevel': 5, 'shuffle': 1, 'blocksize': 0} values=zarr.core.Array>

	0	1
0	538	4
1	538	4
2	541	1
...	...	
146125	540	2
146126	541	1
146127	541	1

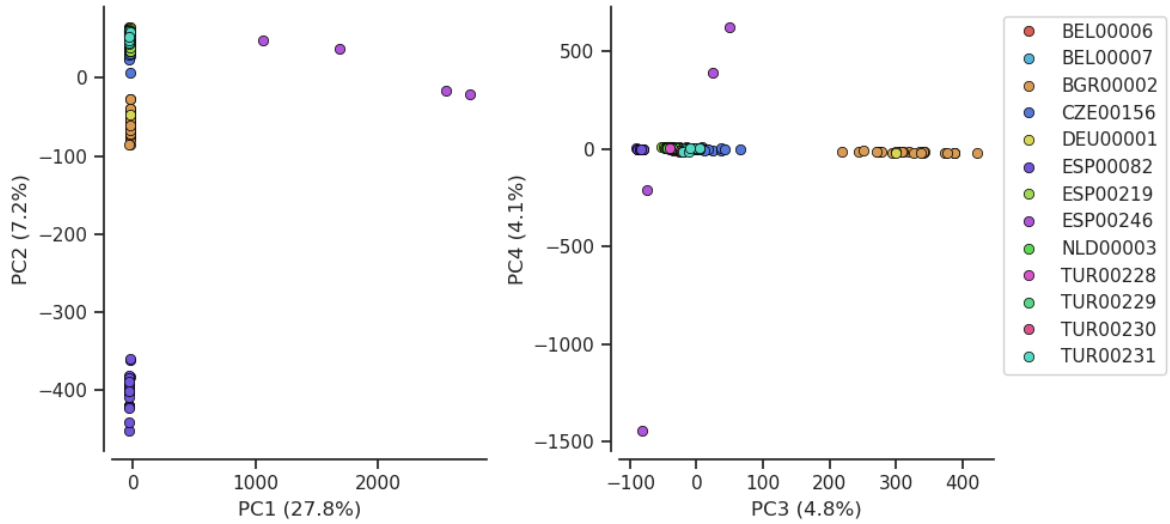
In [77]:
```
flt = (ac2[:, :2].min(axis=1) > 1)
gf = gt_biallelic.compress(flt, axis=0)
gn = gf.to_n_alt()
gn
```

Out[77]:
```
<ChunkedArrayWrapper shape=(106586, 271) dtype=int8 chunks=(3331, 271)
   nbytes=27.5M cbytes=3.5M cratio=7.8
   compression=blosc compression_opts={'cname': 'lz4', 'clevel': 5, 'shu
ffle': 1, 'blocksize': 0}
   values=zarr.core.Array>
```

In [78]:
```
coords1, model1 = allel.pca(gn, n_components=10, scaler='patterson')
```

In [79]:
```
fig_pca(coords1, model1, 'Figure 1. Conventional PCA.')
```

Figure 1. Conventional PCA.



In [81]:
```
outliers = coords1[:,0]>1000
samples[outliers]
```

Out[81]:

	ID	Population
180	ESP00246-006	ESP00246
181	ESP00246-007	ESP00246
196	ESP00246-022	ESP00246
198	ESP00246-024	ESP00246

In [82]:
```
pc_het[outliers]
```

Out[82]:
```
array([41.75791087, 22.82245702, 21.04387934, 40.49395051])
```

In [83]:
```
pc_missing[outliers]
```

Out[83]:
```
array([0.04653455, 0.09991241, 0.04653455, 0.04105989])
```