



Structure Quality Analysis for NAME

Analyses performed for user defined residues.

The constraints analysis is based on the following files: NOE distance constraints file. Angular constraints file. H-bond constraints file.

Procheck analysis,RMSD calculation and structure superimposition are based on: User defined residues

NESG ID: NAME

PDB ID:

Deposition date:

Common Name:

Class:

Length (a.a.): 166

Organism:

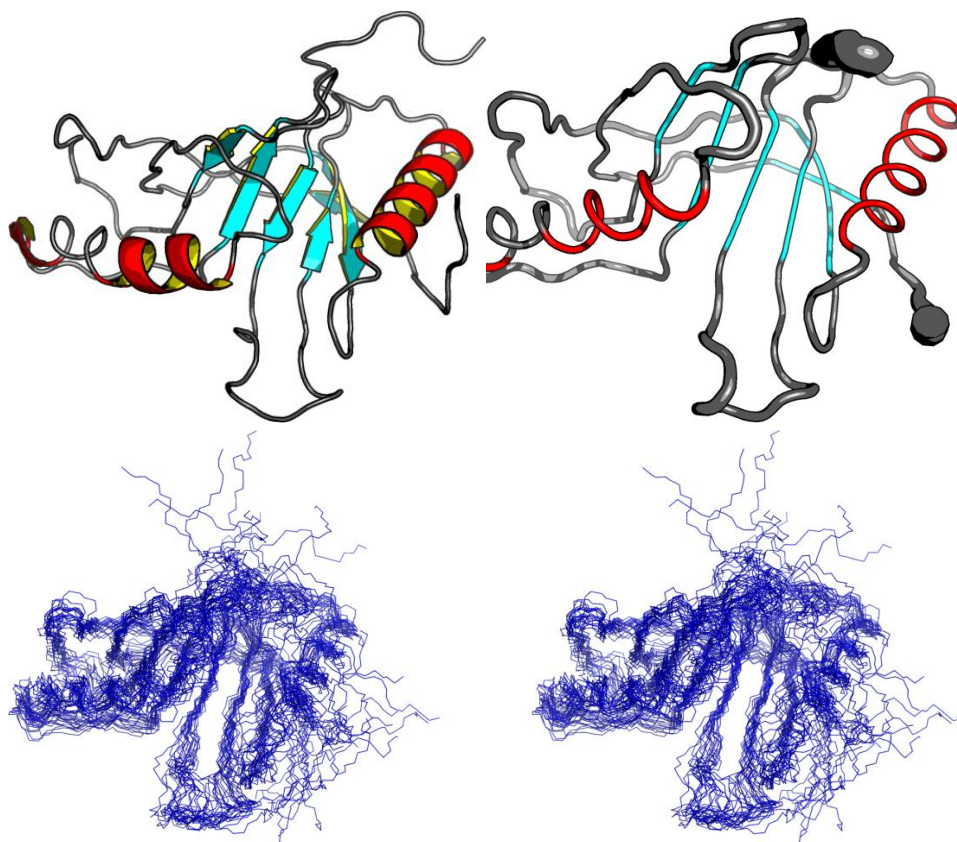
SwissProt /

TrEMBL ID:

models: 20

Oligomerization: monomer

Molecular weight: 18119



Secondary Structure Elements:

alpha helices: 31A-42A, 44A-49A, 109A-122A

beta strands: 10U-14U, 95Y-103Y, 148G-155G, 127U-135U, 58E-62E, 69E-72E, 23G-26G, 75E-76E, 18O-21O, 88L-91L

Total number of restricting constraints per restrained residue: 11.4

Restricting long range constraints per restrained residue: 2.6

Distance violations per model

Calculated using sum over r^{-6}

0.1 - 0.2 Å 0.2 - 0.5 Å > 0.5 Å

7.5 3.65 0.3

Dihedral angle violations per model



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1 - 10 ° > 10 °

5.65 4.2

FIDs deposited in the BMRB? no

RPF Scores

Recall Precision F-measure DP-score

0.968 0.937 0.953 0.722

RMSD *All residues* *Ordered residues*² *Selected residues*³

All backbone atoms 3.7 Å 1.4 Å 1.5 Å

All heavy atoms 4.3 Å 1.7 Å 1.8 Å

Ramachandran Plot Summary for selected residues³ from Procheck

Most favoured regions *Additionally allowed regions* *Generously allowed regions* *Disallowed regions*

96.5% 2.9% 0.0% 0.6%

Ramachandran Plot Summary for selected residues³ from Richardson Lab's Molprobability

Most favoured regions *Allowed regions* *Disallowed regions* [View plot](#) [View model summary](#)

98.9% 1% 0%

Global quality scores

Program *Verify3D* *ProsaII (-ve)* *Procheck (phi-psi)*³ *Procheck (all)*³ *MolProbability Clashscore*

-Raw score 0.42 0.39 -0.11 0.05 6.70

*Z-score*¹ -0.64 -1.08 -0.12 0.30 0.38

Generalized linear model RMSD prediction: 2.21

Close Contacts and Deviations from Ideal Geometry (from PDB validation software)

Number of close contacts (within 1.6 Å for H atoms, 2.2 Å for heavy atoms): 0

RMS deviation for bond angles: 0.7 °

RMS deviation for bond lengths: 0.010 Å

¹ With respect to mean and standard deviation for a set of 252 X-ray structures < 500 residues, of resolution <= 1.80 Å, R-factor <= 0.25 and R-free <= 0.28; a positive value indicates a 'better' score

²Order residues:

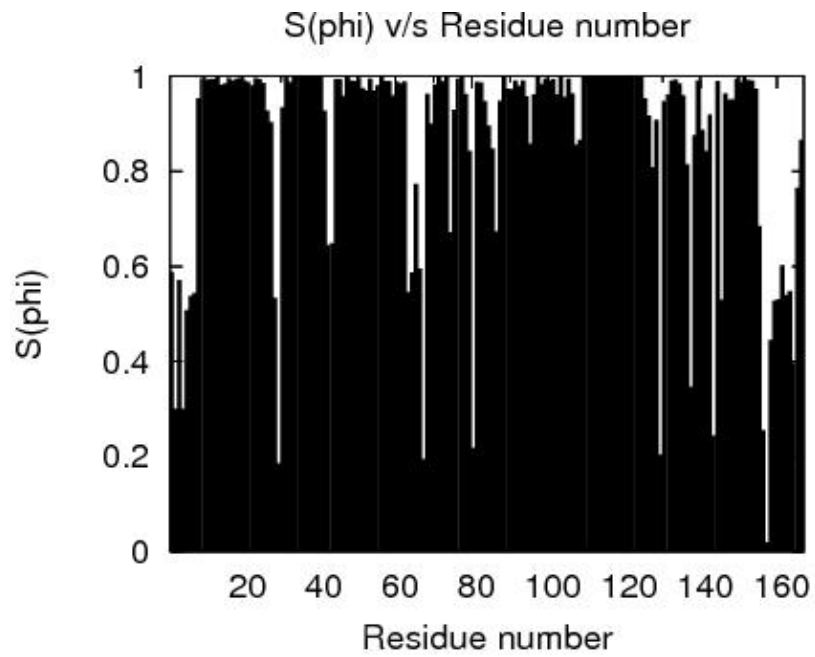
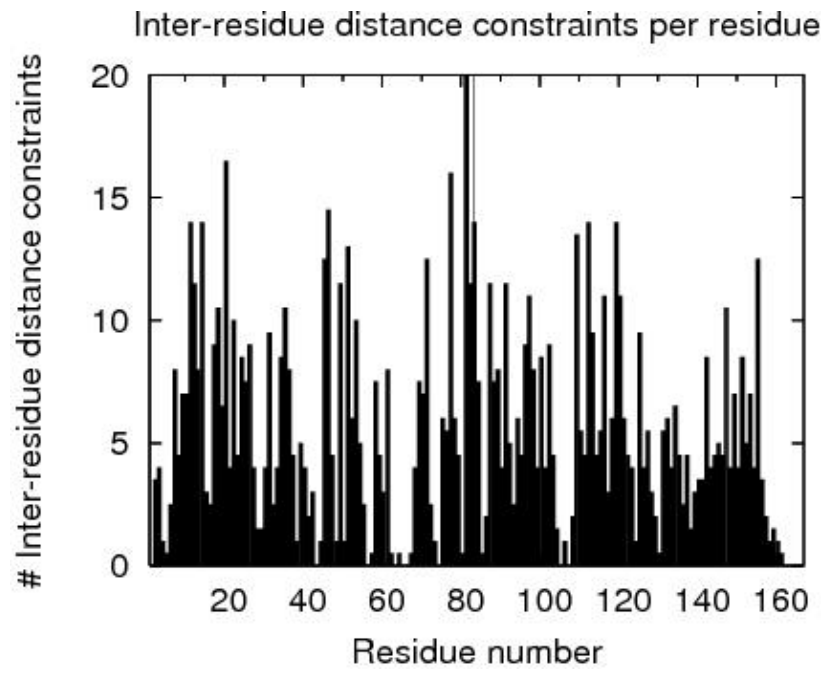
8A-27A,30A-40A,44A-62A,68A-73A,75A-78A,81A-83A,87A-106A,109A-126A,130A-134A,146A-153A

³Selected residues:

8A-27A,31A-40A,44A-62A,68A-73A,75A-78A,81A-83A,87A-106A,109A-126A,130A-134A,138A-140A,146A-153A

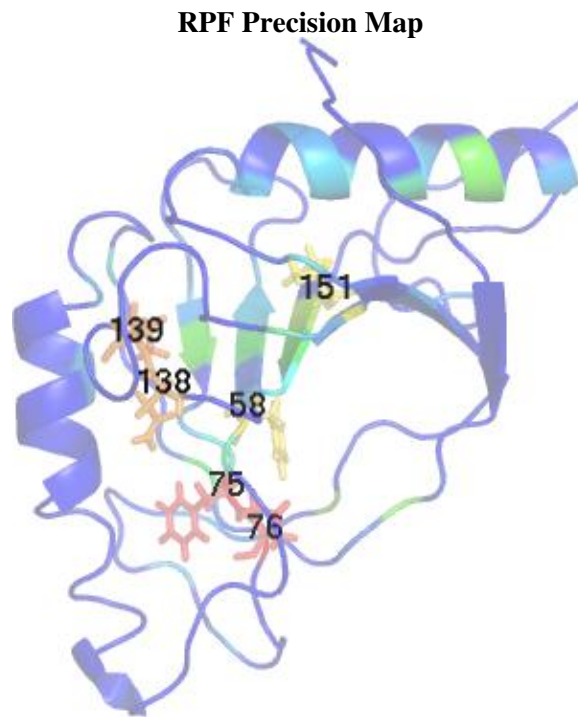
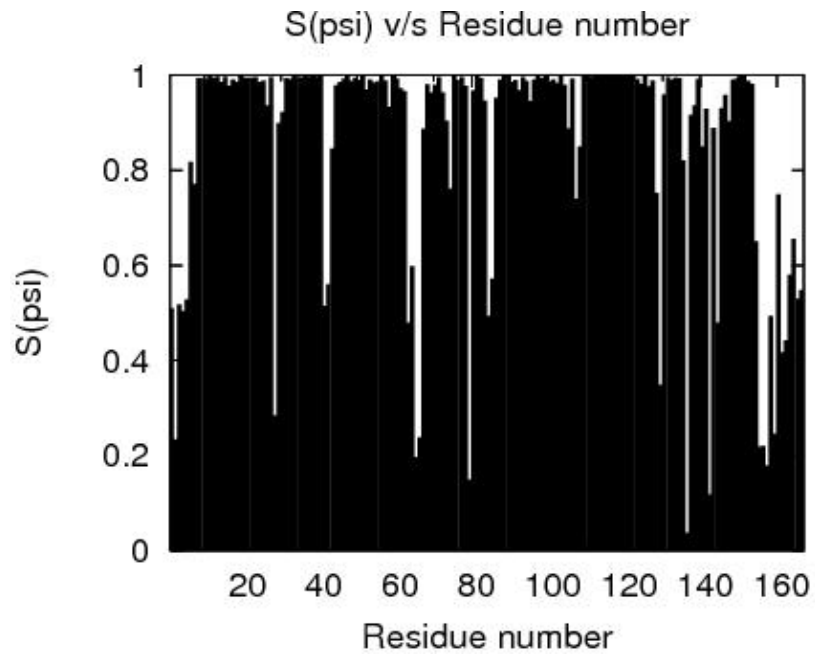


Structure Quality Analysis for NAME





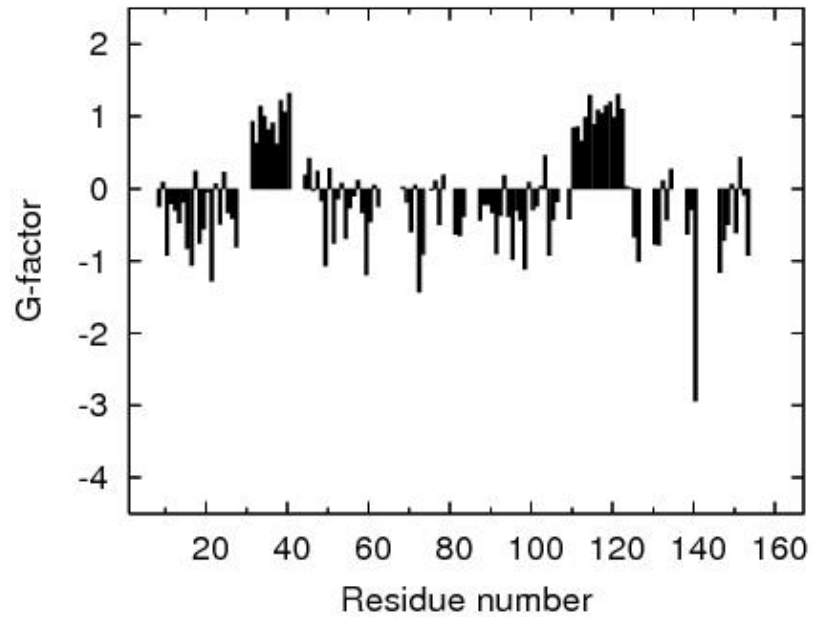
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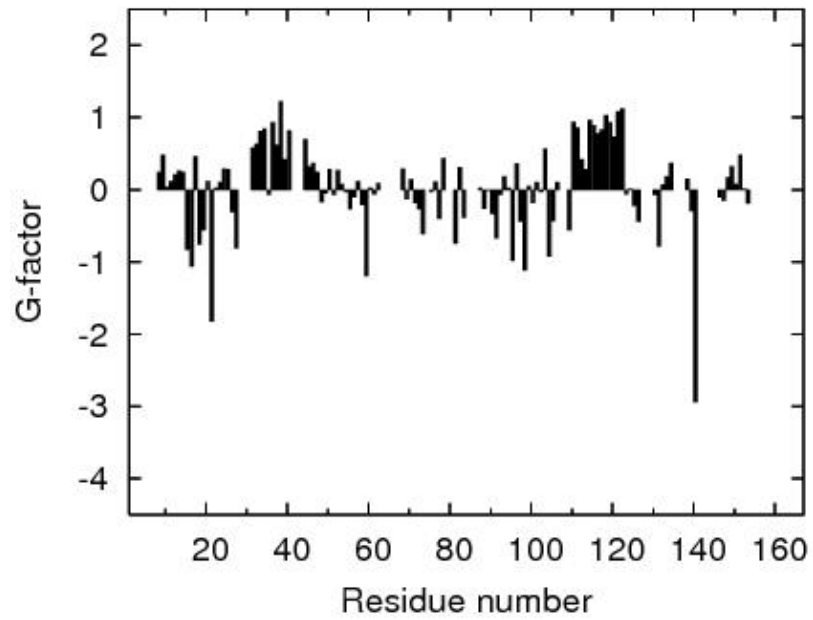


Structure Quality Analysis for NAME

Procheck G-factor for phi-psi

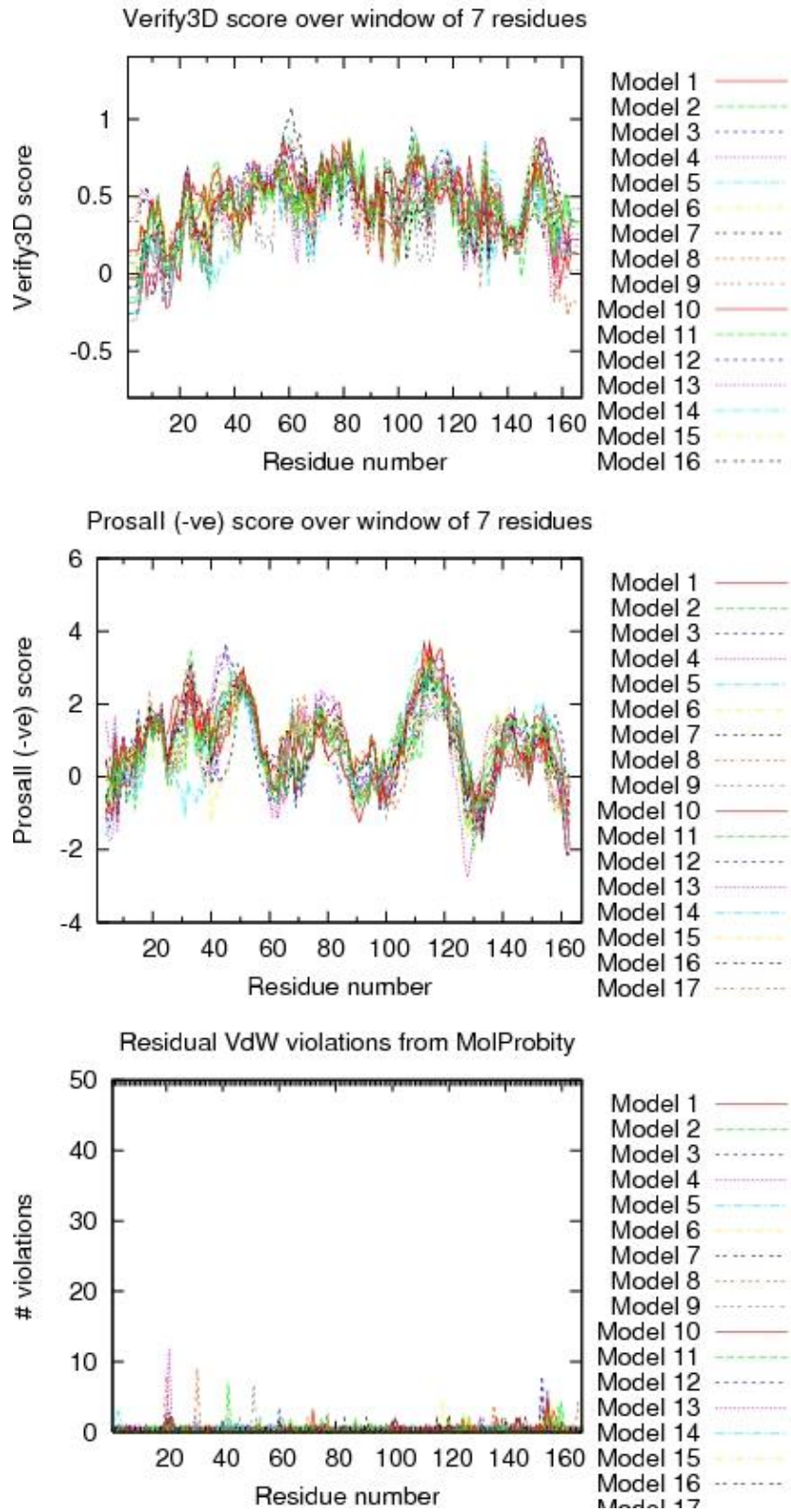


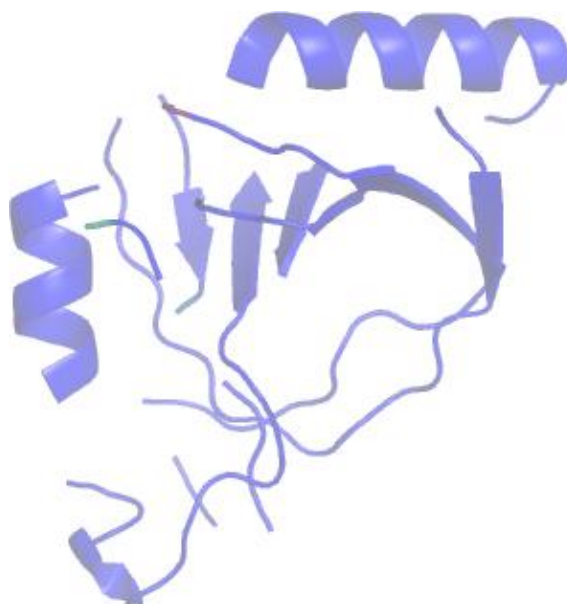
Procheck G-factor for all dihedral angles





Structure Quality Analysis for NAME





Residue Plot of Ramachandran analysis(based on data from Richardson Lab's Molprobit)

References:

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2. Bowie J U, Luthy R and Eisenberg D, "A Method to Identify Protein Sequences that Fold into a Known Three-Dimensional Structure", Science 253 (1991): 164-169
3. Sippl M J, "Recognition of Errors in Three-Dimensional Structures of Proteins", Proteins 17 (1993): 355-362
4. Sippl M J, "Calculation of Conformation Ensembles from Potentials of Mean Force", J Mol Biol 213 (1990): 859-883
5. Laskowski R A et al, "AQUA and PROCHECK_NMR: Programs for checking the quality of proteins structures solved by NMR", J Biomolec NMR 8 (1996): 477-486
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7. Word J M et al, "Exploring steric constraints on protein mutations using MAGE / PROBE", Prot Sci 9 (2000): 2251-2259
8. Word J M et al, "Asparagine and Glutamine: Using Hydrogen Atom Contacts in the Choice of Side-chain Amide Orientation", J Mol Biol 285 (1999): 1735-1747
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10. Tejero R and Montelione G T, "PDBStat", unpublished
11. Luthy R, McLachlan A D and Eisenberg D, "Secondary Structure-Based Profiles: Use of Structure-Conserving Scoring Tables in Searching Protein Sequence Databases for Structural Similarities", Proteins 10 (1991): 229-239
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14. Güntert, P, Mumenthaler, C & Wüthrich, K "Torsion angle dynamics for NMR structure calculation with



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16. Kabsch W, Sander C, "Dictionary of protein secondary structure: pattern recognition of hydrogen-bonded and geometrical features", Biopolymers (1983) 22: 2577-2637

17. Bagaria, A., Jaravine, V., Huang, Y.J., Montelione, G.T., and Guntert, P. "Protein structure validation by generalized linear model root-mean-square deviation prediction". Protein Sci 21(2012), 229-238.

Analysed by on May-9-2013 using PSVS 1.3



Software Environment

Software for structure quality evaluation:

DSSP	DsspCMBI-April-2000
pdbstat	PdbStat-5.4 Version
AutoAssign	Version 2.4.0 (uses only AVS scripts)
RPF analysis	ASDP-1.0
PDB validation	Version 8.061
Verify3D	Version 1.0 corrected by Aneerban
ProsaII	Prosa2003
PROCHECK	Version 3.5.4
MolMol	Version 2K.2

MolProbit programs:

cluster	1999
clashlistcluster	1999 (corrected by Aneerban)
mage	Version 6.35.040409
prekin	Version 6.35.040406
reduce	Version 2.14
probe	Version 2.6

Other Software:

PERL	Version 5.8.0
convert	ImageMagick 5.5.6
ps2pdf	Ghostscript 7.05
htmldoc	v1.9
gnuplot	Version 3.7 patchlevel 3



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jpegtopnm	year 2000
pnmcrop	year 2000
pnmt/jpeg	year 2000