

Appendix E

Positive Matrix Factorization (PMF) Model Parameters

Chemical Species Retained in the Modeling

Ox refers to OCx and Ex refers to ECx for the IMPROVE carbon fractions (these were used in lieu of the NIOSH OC and EC concentration values for this run). Extensive sensitivity studies for the species retained were performed, including but not limited to differences when using NIOSH OC and EC, IMPROVE OC and EC, and IMPROVE carbon fractions. While elements like Hg, Rb and Zr were retained as noted below, they had no effect on the modeled solutions. Also note that species down weighting was performed outside the model through adjustments to the uncertainties, so species were retained as strong.

Species:

Strong ->	O1	O2	O3	O4	
	OP	E1	E2	E3	
	SO4	NO3	NH4	Al	
	As	Ba	Ca	Co	
	Cu	Fe	Hg	K	
	Mn	Ni	Pb	Rb	
	Se	Si	Sr	Ti	
	V	Zn	Zr	PM_coarse	(this was a sensitivity run with
PM_coarse)					
Weak ->	PM2_5				
Bad ->	OC	EC	TC	NIOSH_OC	
	NIOSH_EC	BC	Ag	Au	
	Br	Cd	Cl	Cr	
	Ga	In	La	Mg	
	Mo	Na	P	Pd	
	S	Sb	Sn	Tl	
	Ur	Yt			

Signal to Noise (S/N) Ratio

Signal to noise ratio S/N was evaluated outside of the EPA PMF model and adjusted uncertainties according to the following methodology: The signal-to-noise (SN) ratio was used to screen PM species to be included in the analysis. The SN ratio was calculated by dividing the sum of the values, x_{ij} , that are above the method detection limit (MDL) for a variable j in a sample i by the product of the number of values below the detection limit (BDL), mDL_j , and the MDL [Paatero and Hopke, 2003]. Species with SN ratios between 0.2 and 2 (weak variable) or greater than 2 (good variable) were included in the

analysis, while species with their SN ratios less than 0.2 (bad variable) were excluded. The uncertainties of species with an SN ratio between 0.2 – 2.0 were multiplied by 3 to downweight their role in the mass apportionment. In the carbon fraction data the OP fraction (pyrolyzed organic carbon) was subtracted from the EC1 fraction (the first elemental carbon fraction). To account for this adjustment the EC1 uncertainties were multiplied by 2. For the HI PM2.5 data an analytical uncertainty of 0.8 µg/m³ and MDL of 1.0 µg/m³ were assigned. Analysis of collocated HI PM2.5 mass data collected at the St. Louis – Midwest Supersite showed that precision for these measurements was best represented as an absolute difference (independent of mass concentration) rather than a relative difference.

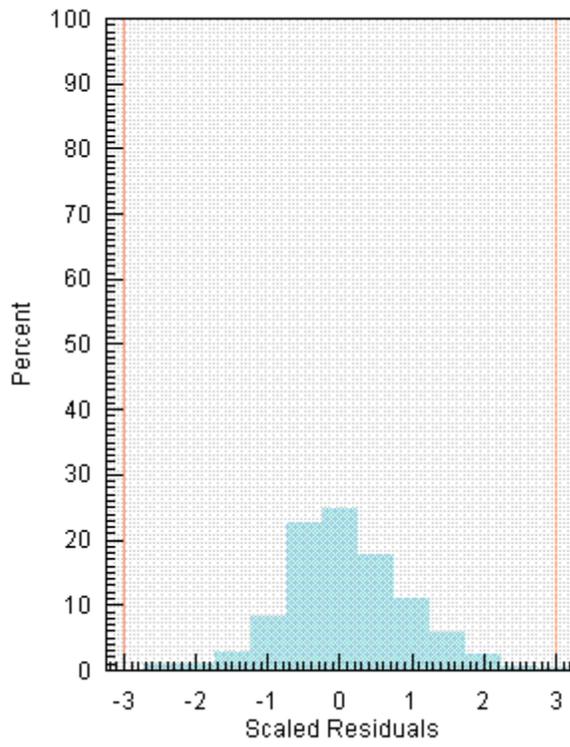
Q-Scores

<u>Q(Robust)</u>	<u>Q(True)</u>	
7404.35	7622.75	(using EPA PMF2)

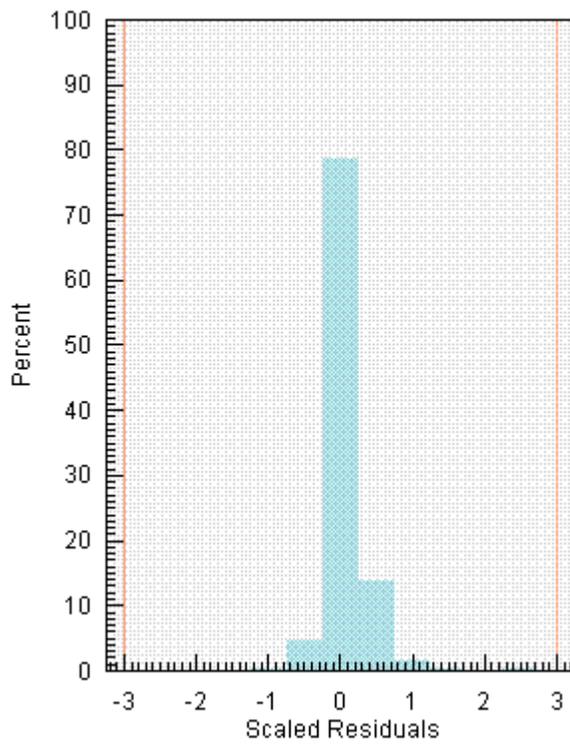
Residuals Analysis

See plots below.

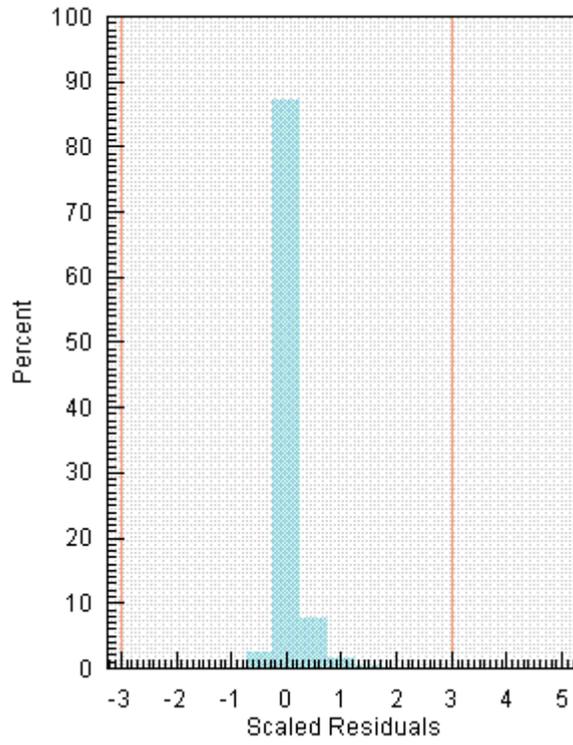
Al



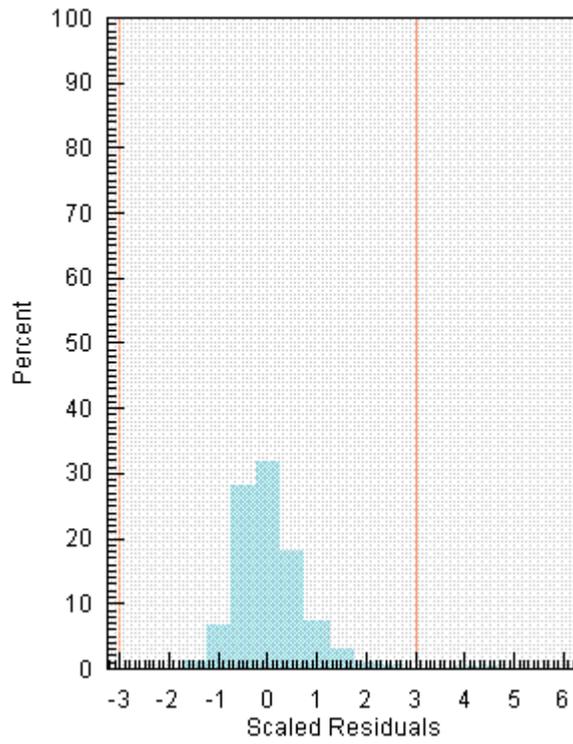
Va



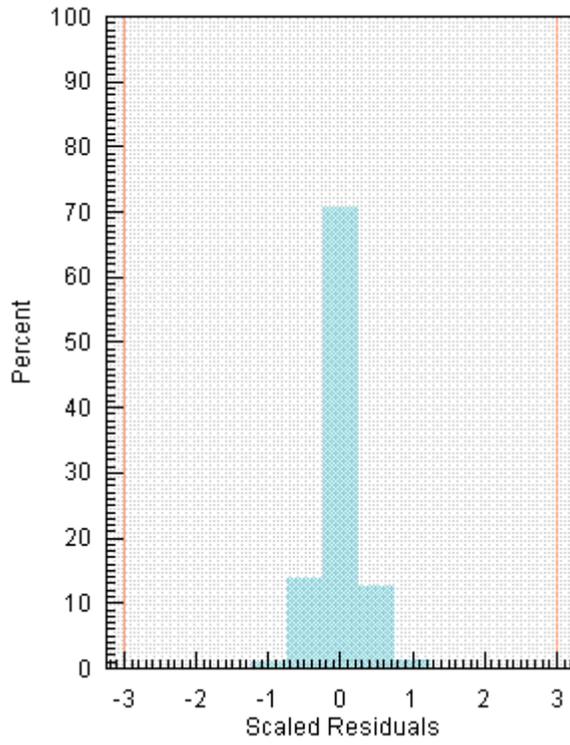
Ti



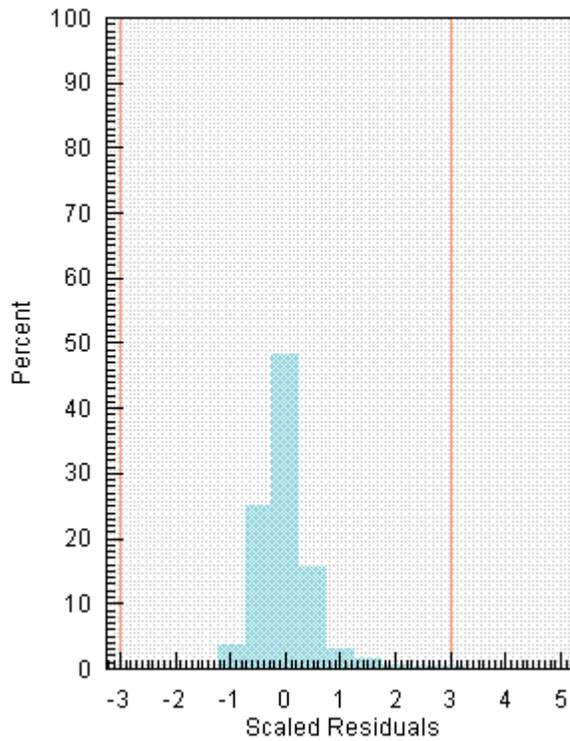
Sr

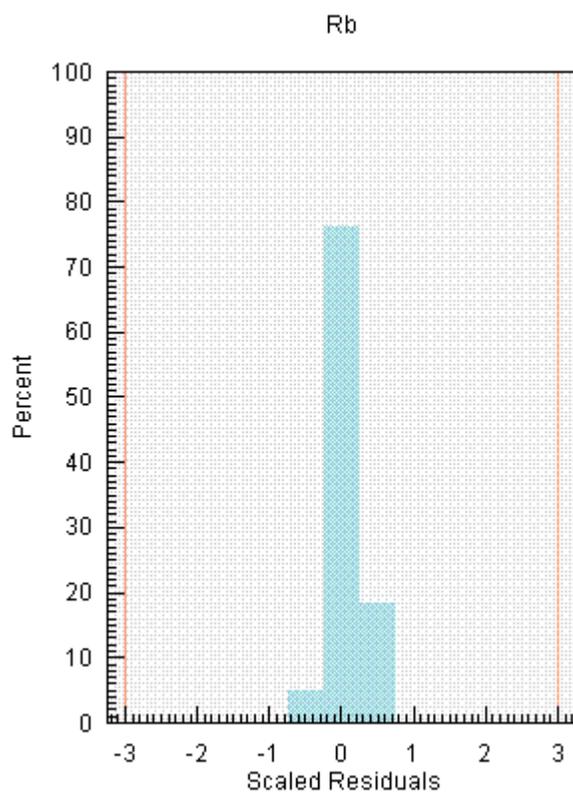
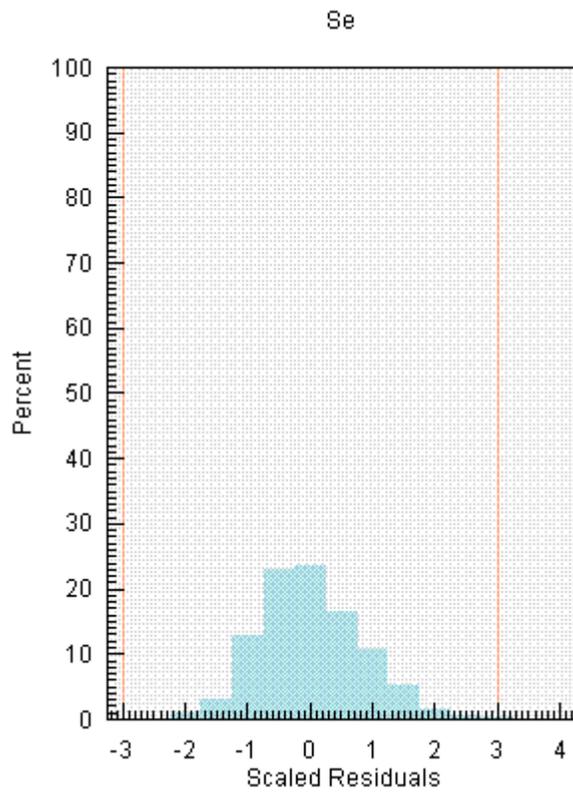


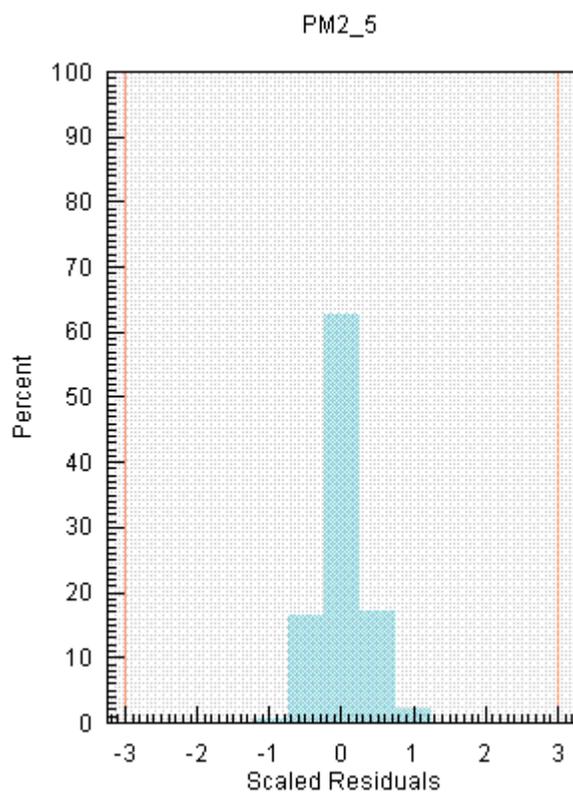
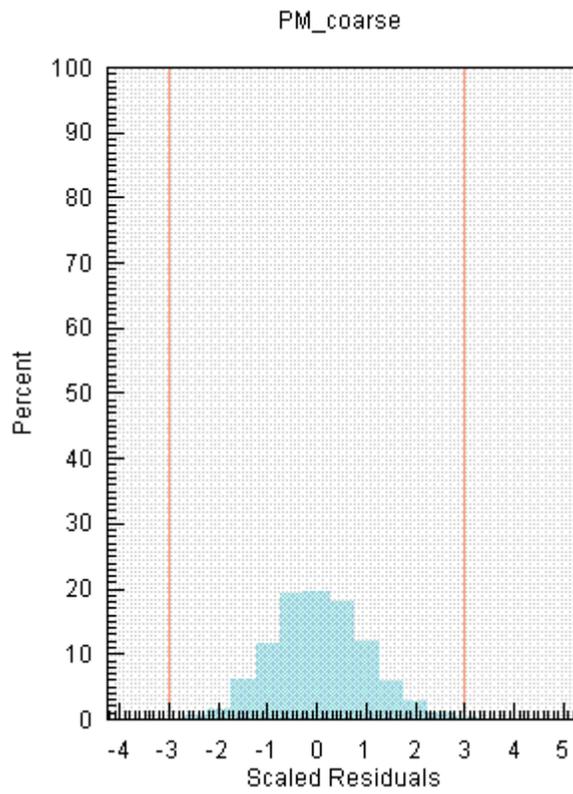
SO4

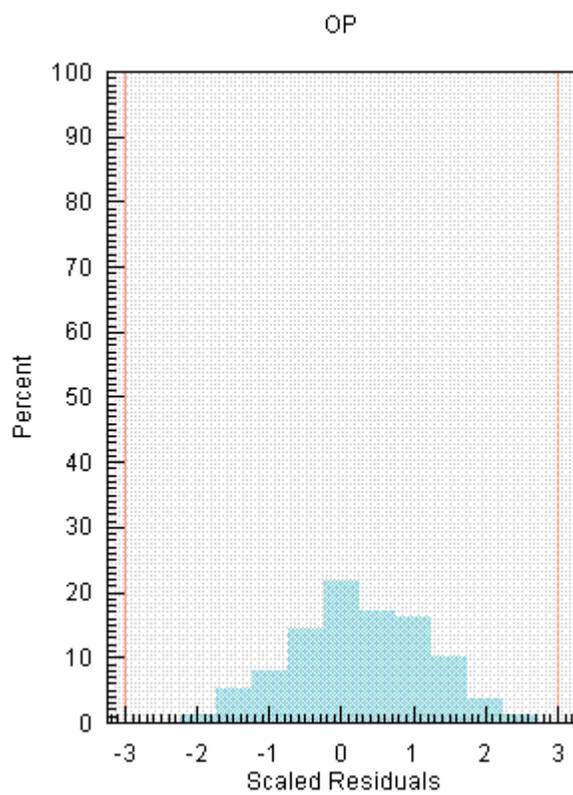
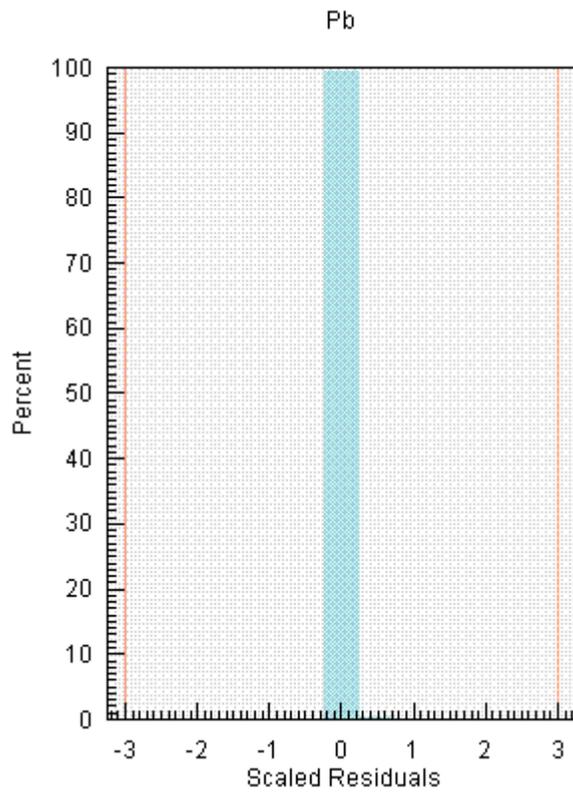


Si

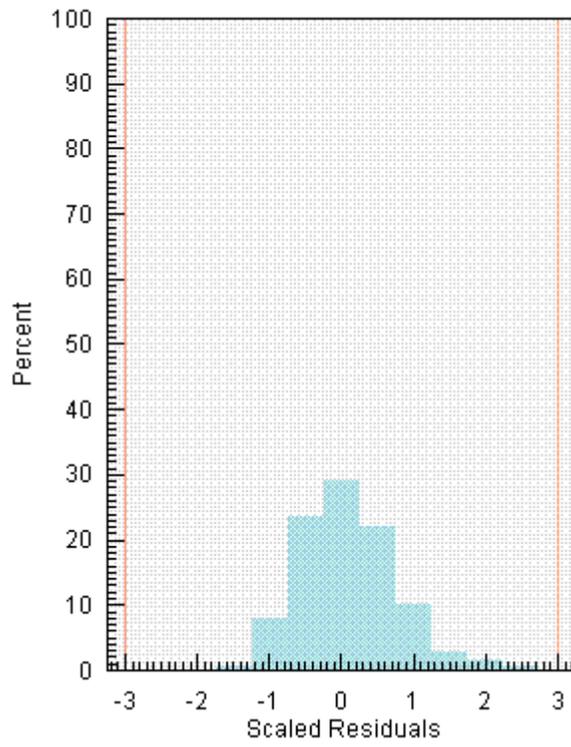




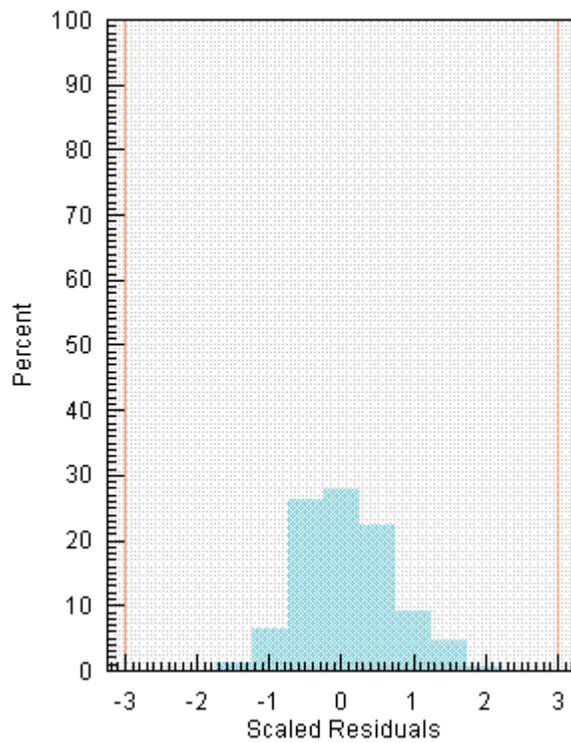




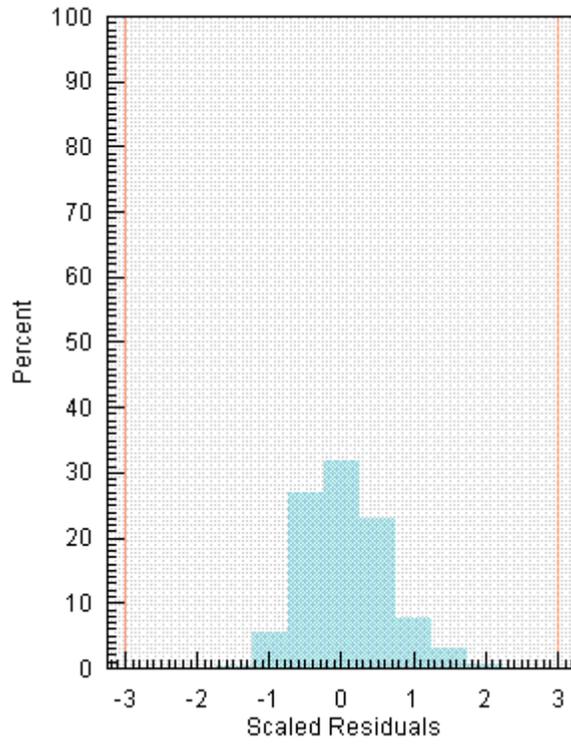
O4



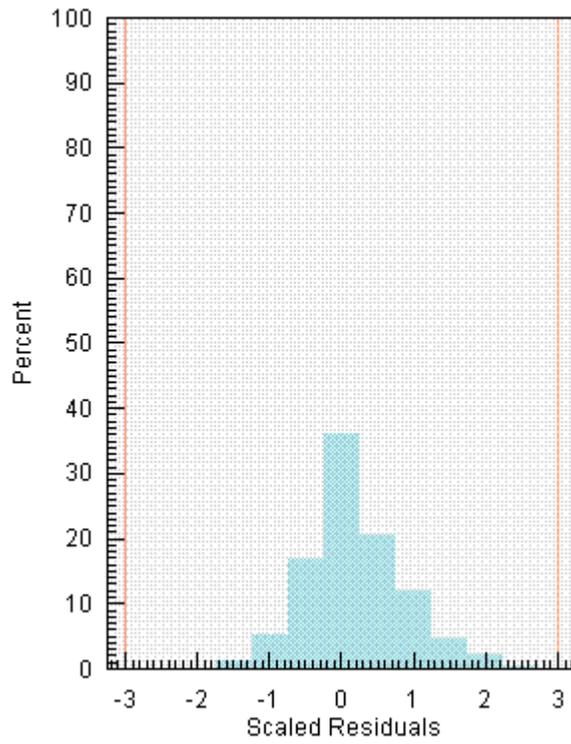
O3



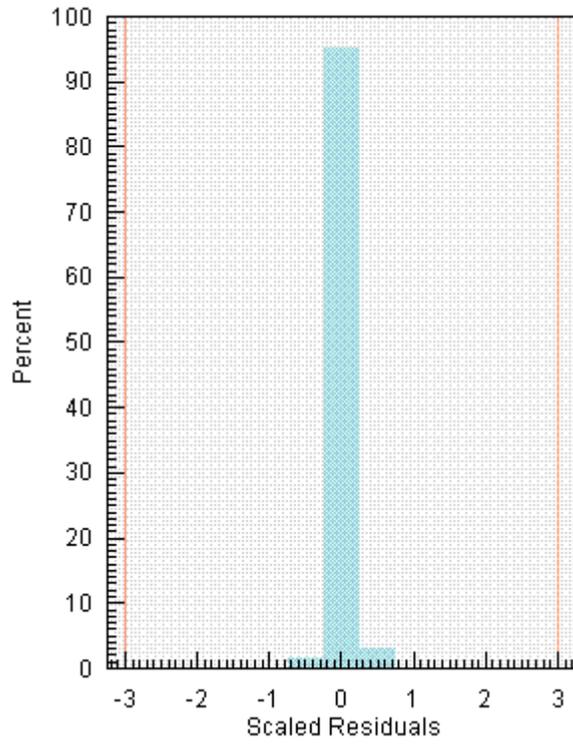
O2



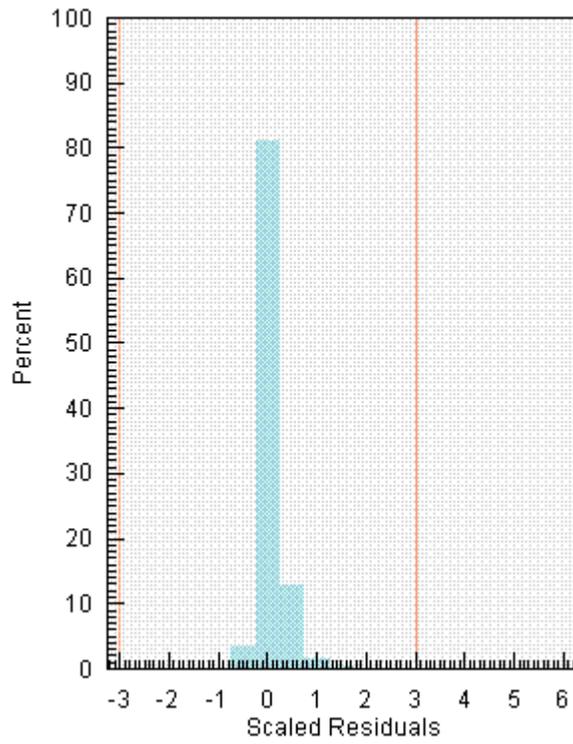
O1



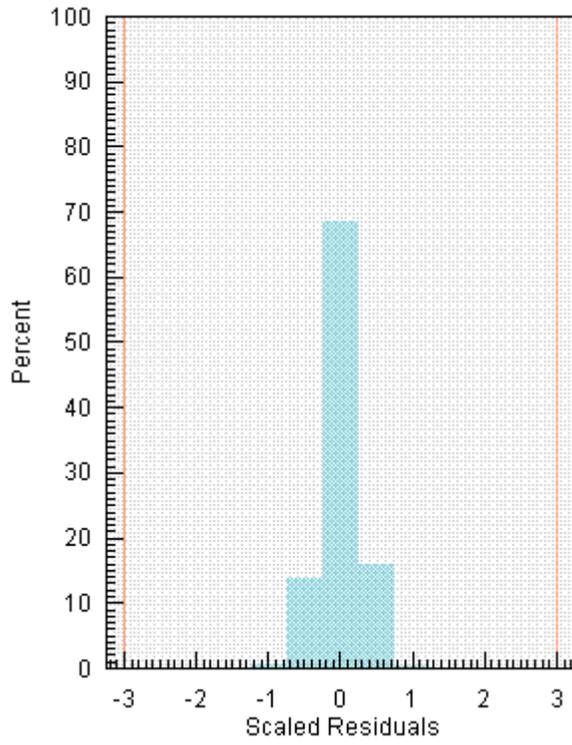
NO3



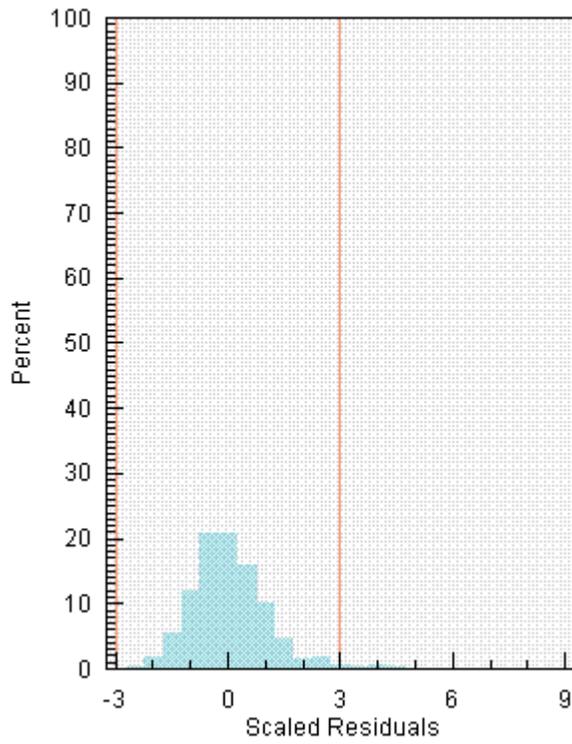
Ni



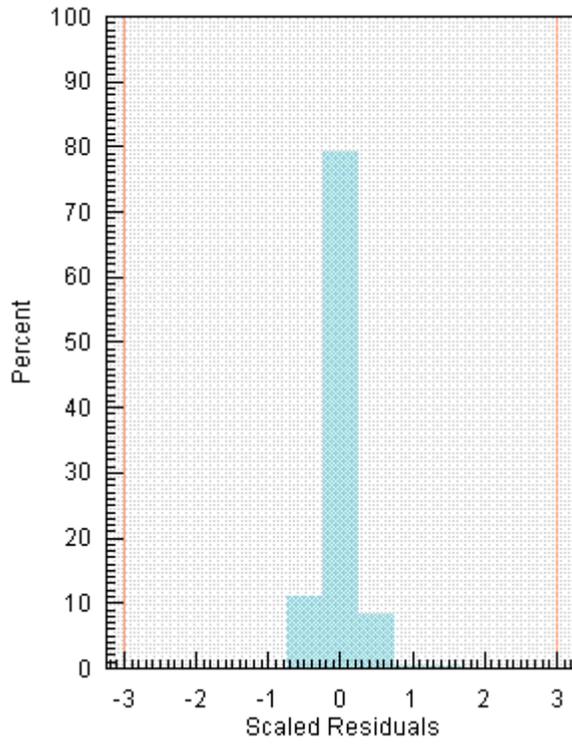
NH4



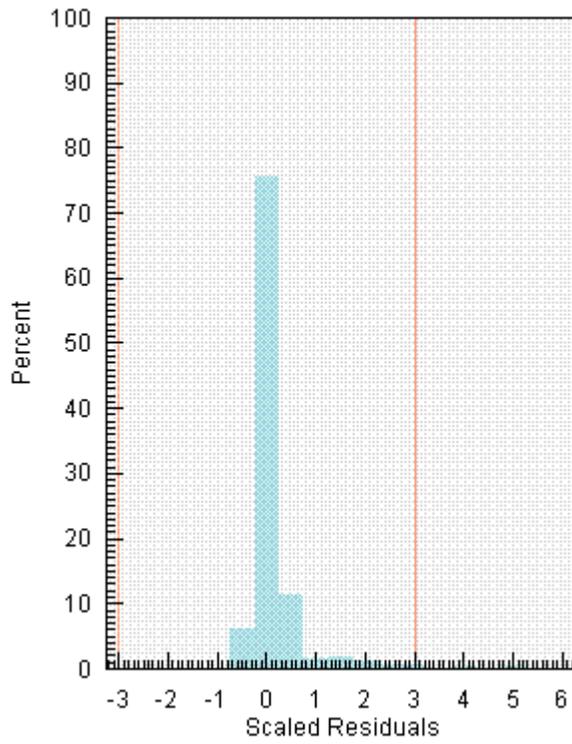
Mn



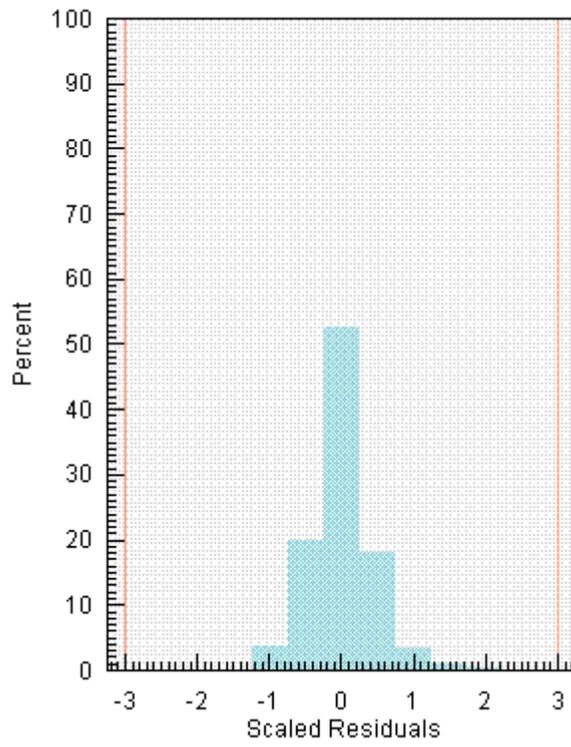
K



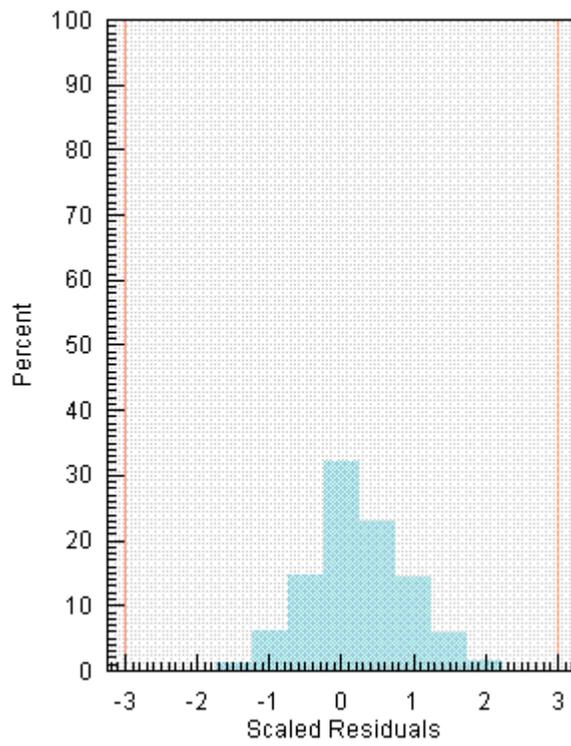
Hg



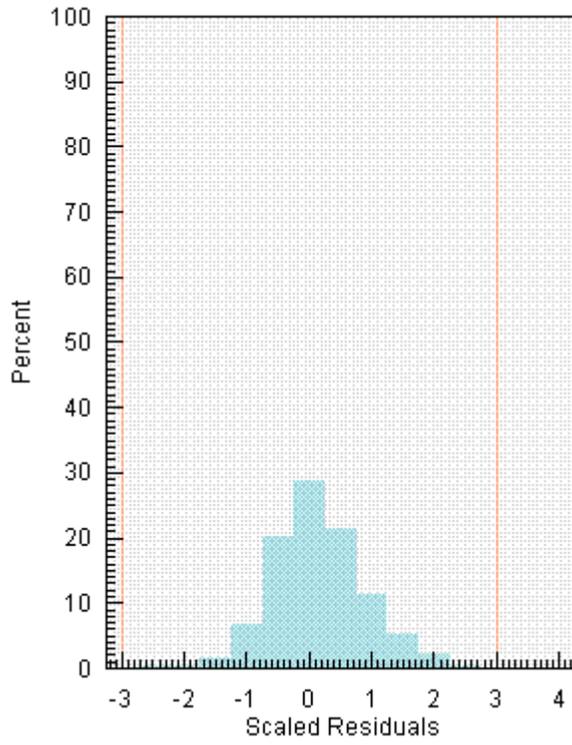
Fe



E3



E2



E1

